UNIVERSITY OF CAMPINAS
SCHOOL OF CHEMICAL ENGINEERING

Christian Carlos Cândido da Silva

Tools for the quick assessment of ideas to improve the energy efficiency in chemical processes

Ferramentas para avaliação rápida de ideias para melhorias em eficiência energética de processos químicos

Campinas
2018

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Dissertação apresentada à Faculdade de Engenharia Química da Universidade Estadual de Campinas como parte dos requisitos exigidos para a obtenção do título de Mestre em Engenharia Química.

Dissertation presented to the School of Chemical Engineering of the University of Campinas in partial fulfillment of the requirements for the degree of Master in Chemical Engineering.

Supervisor: Prof. Roger Josef Zemp, PhD
Co-supervisor: Valdir Apolinário de Freitas, DSc

Este exemplar corresponde à versão final da dissertação de mestrado defendida pelo aluno Christian Carlos Cândido da Silva e orientado pelo Prof Dr. Roger Josef Zemp.

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Alexandre Tresmondi

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Resumo

O trabalho desenvolvido se insere nas áreas de síntese e otimização de processos químicos industriais, com foco em projetos e sistemas que visam à melhoria da eficiência energética dos processos. Foram selecionados alguns tópicos que exemplificam alternativas recorrentes de melhorias em eficiência energética. Foi apresentada uma revisão bibliográfica para cada um dos tópicos avaliados, a fim de localizá-los nas áreas de conhecimento relevantes e indicar as lacunas existentes na literatura. Foram desenvolvidas algumas ferramentas para rápida avaliação de viabilidade dessas opções para melhoria na eficiência energética de processos químicos, a partir de modelos e funções de custo simplificados. As ferramentas desenvolvidas têm o objetivo de auxiliar um engenheiro de processos a percorrer através da árvore de alternativas e descartar rapidamente as inviáveis, evitando assim, despender esforços adicionais em etapas de projeto mais detalhadas. A partir das ferramentas, foram elaboradas análises de sensibilidade assumindo casos-base típicos da indústria química, e finalmente discutidas no sentido de se identificar faixas de viabilidade técnico-econômica e guias para avaliação rápida do potencial de viabilidade dos sistemas estudados.

Palavras-chave: eficiência energética, processos químicos, avaliação técnico-econômica.

Abstract

The work developed lies within the areas of synthesis and optimization of industrial chemical processes, focusing on projects and systems aimed to improving the energy efficiency of processes. Some topics were selected that exemplify alternatives often recurrent in energy efficiency projects. A literature review was presented for each of the topics evaluated, in order to locate them in the relevant areas of knowledge and explicit the gaps in the literature. Some tools were developed to quickly assess the feasibility of these options for improving efficiency of chemical processes, from simplified models and cost functions. The developed tools are intended to assist a process engineer to walk through the tree of alternatives and quickly discard the unfeasible ones, thus avoiding spending additional efforts in more detailed design stages. From the tools, sensitivity analyses were developed, assuming typical cases of the chemical industry, and finally discussed in order to identify technical-economic feasibility fields and guidelines for quick assessment of the potential feasibility of studied systems.

Keywords: energy efficiency, technical-economic assessment, chemical processes.

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Chapter 1

Introduction

The current scenario of industrial competitiveness, increasingly energy costs and tightening environmental regulations make the rational use of energy and the improvement of energy efficiency in chemical processes imperative.

Much has been proposed and done so far to reduce energy costs in the process industries; however, there is still considerable scope to innovate in analysis and design strategies contributing to potential relevant gains in this field. This significant potential scope can be identified when comparing the minimum thermodynamic energy consumption to the actual energy consumption of current processes.

In the realm of a new project, or for a revamp (modification of an existing plant), the role of the process engineer is to evaluate the available technologies to perform a given task and decide the alternative that best meets the technical and economic criteria.

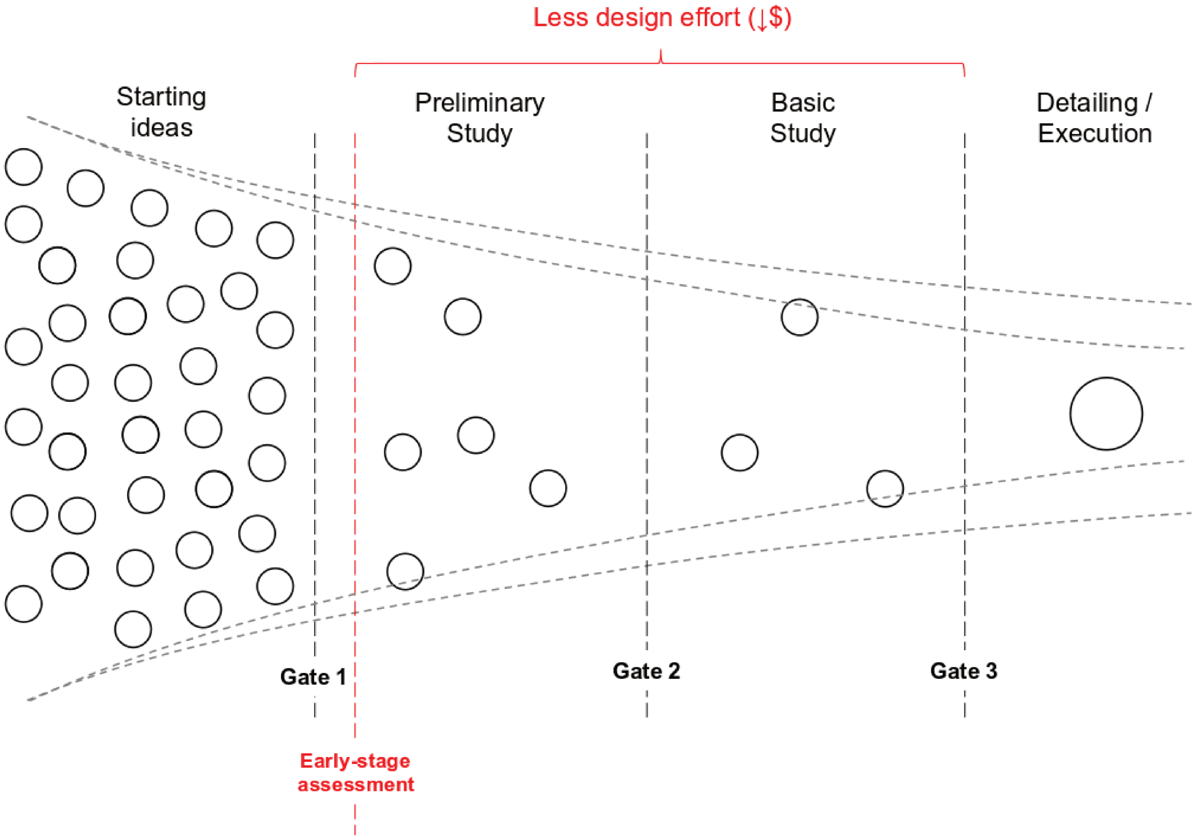
In the case of a new project, the process engineer is faced with a large number of technology options and ways to define the best process, which should present a trade-off between investment cost and resource utilization. In the case of an existing plant, it is intended to identify changes which have key impact on process energy efficiency. In this context, the process engineer must evaluate modification options and their impacts in a holistic way.

1.1 Knowledge area

This work is located in the areas of synthesis and optimization of industrial chemical processes and it contributes to the current methodology of assessment of chemical process elements, at early stages of the process development, through low-complexity models, taking into account its technical and economic feasibility.

During process synthesis, the design team is faced with several options and alternative technologies for a given process element. These options are dropped as the project becomes more mature and more information is available. A project develops itself during some steps with growing details and accuracy; these stages undergo validation gates and allow the proceeding to the corresponding next step. The typical gates and maturity stages of a project are shown in Figure 1.1.

Figure 1.1: Maturity evolution of a project



A common challenge during the study of processes is the evaluation of the economic feasibility to support the decision to continue or not with the study. The evaluation of the feasibility of an energy efficiency project, for example, in early stage is a challenge since it depends on information that is not available in a superficial and initial approach. The tools developed in the present work should help the engineer to run through alternatives tree and quickly discard unfeasible ones, and thus avoiding spending additional design efforts and associated costs.

Projects often involve a trade-off between investment cost and operating costs (or gains). It must be kept in mind that deviation of the actual energy consumption from the optimal consumption in a process is due to the second law of thermodynamics, in other words, irreversibilities which are intrinsically derived from driving forces imposed by finite heat exchanges, not resisted expansions, friction and uneven chemical potential interactions.

This work will study some systems and unit operations which compose a whole industrial chemical process and their interactions. These processes include reactions (chemical transformations), separations, heat exchange, fluid transport and utilities allocation.

For all those systems a simplified model, computational tools and a economic evaluation for equipment and / or systems will be developed.

1.2 Objectives

This work aims to contribute to build directives for technical and economic assessment based on the development of simplified models and computational tools of some ideas for improving energy efficiency of chemical processes.

This contribution, although modest, can ultimately help on the evaluation and screening of projects in early stages of development and/or when little information is available. This will be done through:

- Review of some currently available best technologies and practices regarding energy efficiency projects for chemical process industries;
- Development of seven simplified models for quick technical and economic evaluation, as listed in the following chapter;
- Development of tools and guidelines to assist the selection of technological options and the conception of ideas of energy efficiency improvement projects;
- Development and enumeration of some policies and practices promoting the rational use of energy resources by the process.

Process design at early stage demands that several ideas to be evaluated quickly in order to support go / no go decisions, for projects for both new and existing processes.

The main target audience of this work is the process engineer and other professionals who deal with conception, specification and cost estimation of projects on energy efficiency in chemical processes. These professionals often face the need of quick screen a considerable number of project alternatives and to select a few of them or at least determine priority to keep alternatives for further project specification and detailing.

1.3 Limitations

This work is not intended to be used on detailed design stages of project, but for comparative assessment between technology options in early stage of process design.

The models listed here are shortcut methods, for quick calculations while little information is available.

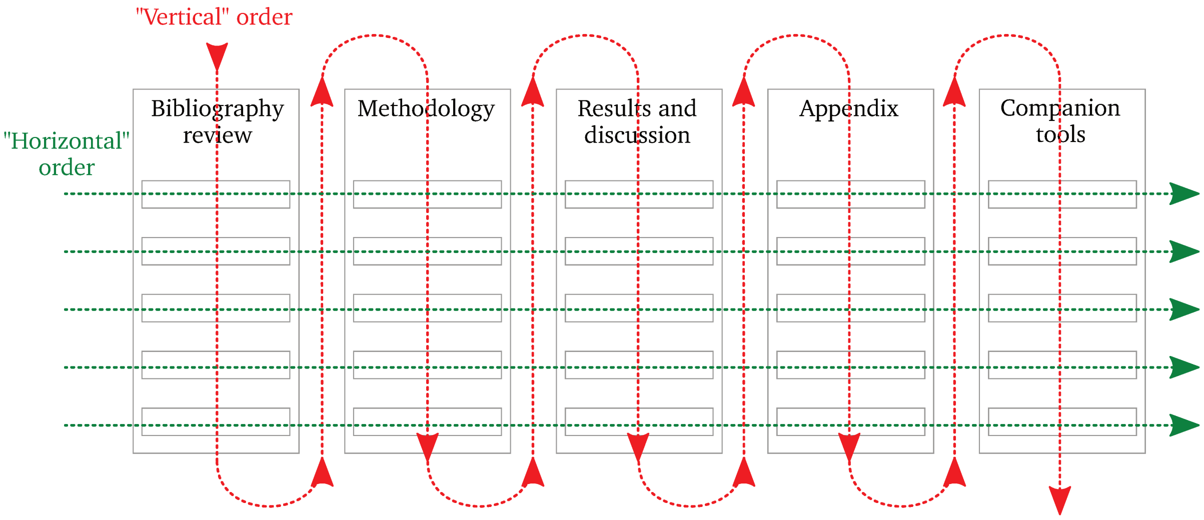
1.4 Structure of this work

This work is structured in 5 main chapters: Introduction, Literature review, Methodology, Results and Discussion and Tools screens.

Except for the Introduction chapter, all the others are subdivided with the same numbering schema, as can be seen in the Figure 1.2.

For example, the subject which was reviewed in the section 2.**3.1**, have its models described in the section 3.**3.1**, results in section 4.**3.1**, appendix A.**3.1** and companion tool number **3.1**.

Figure 1.2: How this work is structured and alternative reading orders for this work



In other words, the are two different ways of reading this work. The traditional one, which goes through the document “vertically”, one chapter after another, or the “horizontal” order, which will consider only the subject of interest, as shown in Figure 1.2.

Chapter 2

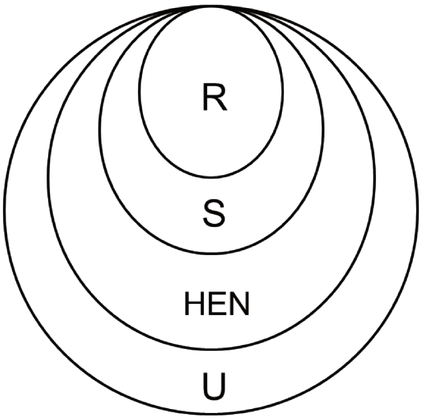
Literature review

2.1 General literature review

The structuring of the work followed the general structure of process design described by Douglas (1985, 1988), where the definitions during project goes from the reaction system, separation systems, heat exchange networks, ending with utilities allocation.

Smith and Linnhoff (1988) published a layered overall process design concept named "onion model", where the project design develops itself from the inner layers to outer ones, which are hierarchically dependent. Figure 2.1 illustrates this conceptual structure.

Figure 2.1: The layered process design "onion" diagram



Source: Adapted from Smith and Linnhoff, 1988.

The letters in the drawing stands for R – Reaction, S – Separation, HEN – Heat

Exchange Network and U – Utilities system.

Following this hierarchical structured plan for decision-making process, it is intended to assess, at each level, conditions, variables and basic parameters which allow discrimination among technology alternatives and determination of their acceptance or rejection.

A trade-off approach for feasibility analysis, based on the second law of thermodynamics, was tackled by Steinmeyer (1982, 1988, 1992), but it remains incomplete in respect to a more fundamentally and holistic approach. It is in this gap that this work aims to contribute, considering real life cases coupled with fundamental technical-economic analysis.

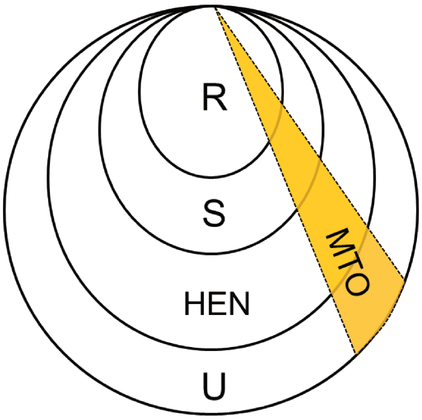
As far as we know from the technical and scientific literature, there is no availability of a approach based on simple models in order to identify technology options to improve energy efficiency in chemical processes from a technical and economic point of view.

The “missing” layer

Momentum Transfer Operations (MTO) are not covered in the original “onion” model, but still they are a fundamental element of chemical processes and must not be neglected during process synthesis steps.

To address this weakness, momentum transfer systems were included on the analysis of this work and included as an onion slice, as shown in Figure 2.2, because these operations permeate over all onion layers and must be accounted during every process design step.

Figure 2.2: The “onion” diagram including the slice of momentum transfer operations



To the best of our knowledge, no previous work has attempted to revise process elements, apparently disconnected from each other, that add up to chemical processes, in addition to the classical elements: reactors, separators, heat exchangers and pumps.

On the following sections, some introduction, definition and specific literature review can be found for each studied system, following the layers of the onion model.

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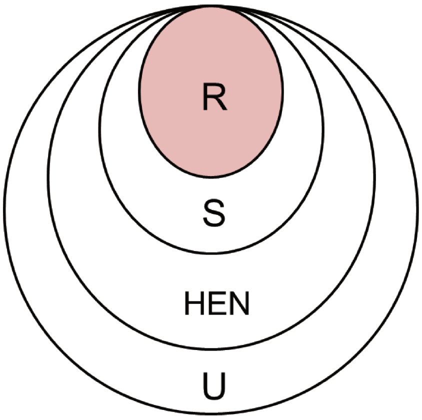
2.2 Reaction



2.2.1 Specific energy consumption in chemical processes

(Paper submitted to Chemical Engineering Progress in December 2017)

Energy use is a relevant component for the economic feasibility of chemical processes and products because it can reach relevant shares of production costs. Quick estimates of the energy use at very early design stages of new processes and products is important to guide decisions through effective screening and selection procedures.

These estimates can be done by considering typical shares of energy in the costs of chemicals or by considering the relations between enthalpy of reaction ($\Delta H^\circ_\mathrm{R}$) and the *Specific Energy Consumption* [1] (SEC) of a manufacture process.

Although both approaches cannot be precise at early stages of development and design, the SEC x $\Delta H^\circ_\mathrm{R}$ approach can be more advantageous because, by using a fundamental process parameter, it can make direct inferences in a spectrum of products. Furthermore, an early estimate for the energy intensity of a new process is also important to prospect its environmental impact in terms of carbon emissions, provided the shares of the energy sources and types used are known.

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[1] The total energy required to produce a given amount of product, including thermal, chemical and electrical forms of energy. It is well known that energy cannot be "consumed", and a more appropriate term would be energy "use", however, we will take permission to use here the term "consumption" due its wide use in the literature.

This work revisits and reviews the approach for the estimation of SEC of a chemical process based on early information of synthesis paths: the enthalpy of reaction ($\Delta H^{\circ}_{\mathrm{R}}$) and the variation of the specific Gibbs free energy ($\Delta H^{\circ}_{\mathrm{G}}$) due to reaction.

Previous work

Not much work has been published in literature aiming the prediction of the overall *Specific Energy Consumption* (SEC) of industrial chemical processes. Thus, the known approaches correlating SEC with thermodynamic functions of chemical products are revisited here.

Bridgwater (1975) proposed a function correlating the specific energy cost and the number of functional units, capital cost and capacity of chemical plants. Process parameters, such as the enthalpy of the reaction, were not taken into account.

Bridgwater suggested that there was scope for improvement of correlations in this direction recognizing that correlations taking into account the thermodynamic characteristics of chemical reactions would be more accurate and more grounded in basic process parameters. Advancing in this direction, Sommerfeld and White (1979) proposed a correlation between the specific consumption of chemical facilities and the enthalpy of reaction of base chemical and petrochemical processes.

The work of Sommerfeld and White (1979) remained as the only approach available to estimate SEC at early stages of process design until when Lange (2001) presented a plot of the SEC versus the enthalpy of reaction for a set of base chemicals and petrochemicals. Lange didn't propose a correlation for his plot, but concluded that chemical processes could amount energy consumption up to 25 MJ per kg of product, depending on the enthalpy of reaction of the involved synthesis.

Lange (2001) obtained results similar to those of Sommerfeld and White (1979) correlating the SEC to the enthalpy of reaction for several base chemicals and petrochemical processes (apparently in independent manner as the work of Sommerfeld and White is not mentioned).

Later on, aiming to identify the sources of thermal losses in batch chemical processes, Bieler *et al.* (2005) published data on the specific steam consumption of 15 undisclosed chemical specialties, along with their respective enthalpy of reaction. No correlation was proposed.

Neelis *et al.* (2005), intending to analyze the sustainability and emissions of greenhouse gases for several chemical processes, published a collection of energy indicators, among these the SEC and $\Delta H_{\mathrm{R}}^{\circ}$. Similarly to Sommerfeld and White (1979) and Lange (2001), Neelis *et al.* suggested that chemical processes can reach energy consumption up to 20 MJ/kg above the enthalpy of reaction.

Bumann *et al.* (2010) proposed a method for estimating the SEC at early stages of chemical process design based on process parameters. Besides the enthalpy of reaction, process parameters such as the reaction temperature, enthalpy of vaporization and products concentrations in reaction step are taken into account. This approach seems to be more accurate, but certainly requires more information than the previous approach correlating only SEC and $\Delta H_{\mathrm{R}}^{\circ}$.

Another collection of SEC for several products was is found in US Department of Energy (DoE) (2015), where several basic chemicals and petrochemicals were listed along with their SEC reported in the literature and their theoretical minimum energy consumption, based on the variation of the specific Gibbs free energy due to reaction ($\Delta G_{\mathrm{R}}^{\circ}$). No correlation between SEC and $\Delta H_{\mathrm{R}}^{\circ}$ was proposed.

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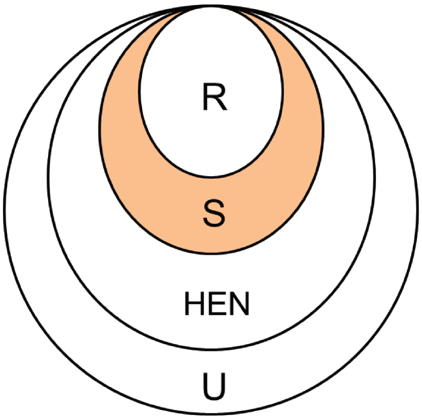
2.3 Separation operations

Separation operations consist on the promotion of formation of two or more phases from a mixture, in order to obtain one or more components of the mixture separately. Here are included solid-fluid, solid-solid and immiscible and miscible liquid-liquid separation, including distillation, which is still responsible for a large share of energy consumption in chemical industry.



2.3.1 Heat pump assisted distillation

Heat pump aided distillation process consists on the application of a heat pump to upgrade and recover the available condensing heat of column overhead stream and use it on the reboiler.

Heat pump assisted distillation can achieve savings from 20% up to 50% when compared with conventional distillation.

Kiss *et al.* (2012) reviewed about the available technology options for efficient distillation, with focus on heat pumps. According to Kiss *et al.* (2012), the Mechanical Vapor Compression (MVC) distillation is one of the most promising and feasible (technical and economically) technology.

In this work, we will study only this specific heat pump technology and to assess how the economic feasibility varies with process parameters and requirements.

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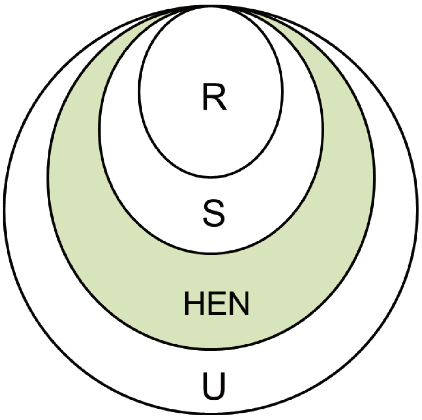
2.4 Heat transfer operations

Heat transfer operations consist of unit operations which promote heat exchange between two or more streams, directly or indirectly through a heat exchanger.



2.4.1 Thermal Integration

One of the most typical targets for thermal energy savings projects is the heating and cooling processes in heat exchangers, using utilities.

The adoption of energy integration to reduce the demands of utilities has existed since the beginning of the chemical process industry, but has been disseminated only after the advent of the *Pinch technology* proposed by Linnhoff *et al.* (1982), which established a systematic and accessible way of identifying the minimum utility consumption targets and which assists on the construction of heat exchangers networks for thermal integration.

Fundamentals and the state-of-the-art on heat integration can be found elsewhere (see SMITH, 2005 and KEMP, 2007).

Several studies have been published on systematic generation of heat exchanger networks and energy targeting using mathematical programming and automated heuristics (see PONCE-ORTEGA, 2010 and SHORT, 2016), however those procedures take more time and resources than one is willing to take during a approach study.

Unfortunately, a heat integration exchanger network that gets close to the energy targets is often not economically feasible. This forces the engineer to accept a higher operating cost with utilities in exchange for a lower investment cost in heat exchange equipment.

As far as we know, no published work have tackled heat integration focusing on single heat integration exchanger. In this work we focus on this gap.

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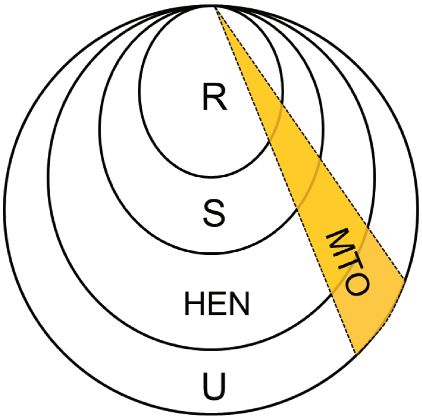
2.5 Momentum transfer operations



2.5.1 Pumping systems

Liquid pumping systems are ubiquitous in chemical process plants and pipeline transport.

The currently available recommendations in the literature, often addressed in "rules of thumb" and "economic velocities" are immutable for years.

Some recommendations for piping design based on mean fluid velocity are available in engineering literature, such as:

- 1.5 - 3 m/s for water (average service) (HALL, 2012)
- 1 - 3 m/s for water of fluid similar to water (PETERS and TIMMERHAUS, 2002)

The current work aims to recheck these assumptions and assess the sensibility of these recommendations in respect to fluctuations and long term variation on energy and capital costs.

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2.5.2 Steam turboexpansion

In a industrial steam network, processes require that heat be supplied at different temperature levels, and this requires complex pressure reduction networks after the generation of steam centralized in a boiler.

Expansion of steam can be done properly in a reducing valve, but the unresisted nature of the expansion transforms a potential pressure power into heat, which could be used to run a heat engine and generate useful work.

In this sense frequently arise the alternative to perform the service of reduction in a steam turbine (turboexpander) in order to take advantage of the lost work and to generate electrical energy or to turn rotary machines and the technical-economic feasibility of this alternative.

Harrell and Jendrucko (2009) made a review of the main parameters and models to help on the assessment of a steam turbine in place of a valve.

A important factor that have been hindered set-ups of this kind is the historically low efficiency of the smaller steam turbines, that would be used to replace local steam reductions.

Some high-efficiency have become commercially available in the last years (see SPIRAX-SARCO and CARRIER), the said "microturbines" can give high isentropic efficiencies, comparable to large turbines

This work aims to contribute giving some useful sensitivity analyses to help an early stage assessment of this alternative.

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2.5.3 Steam thermocompression

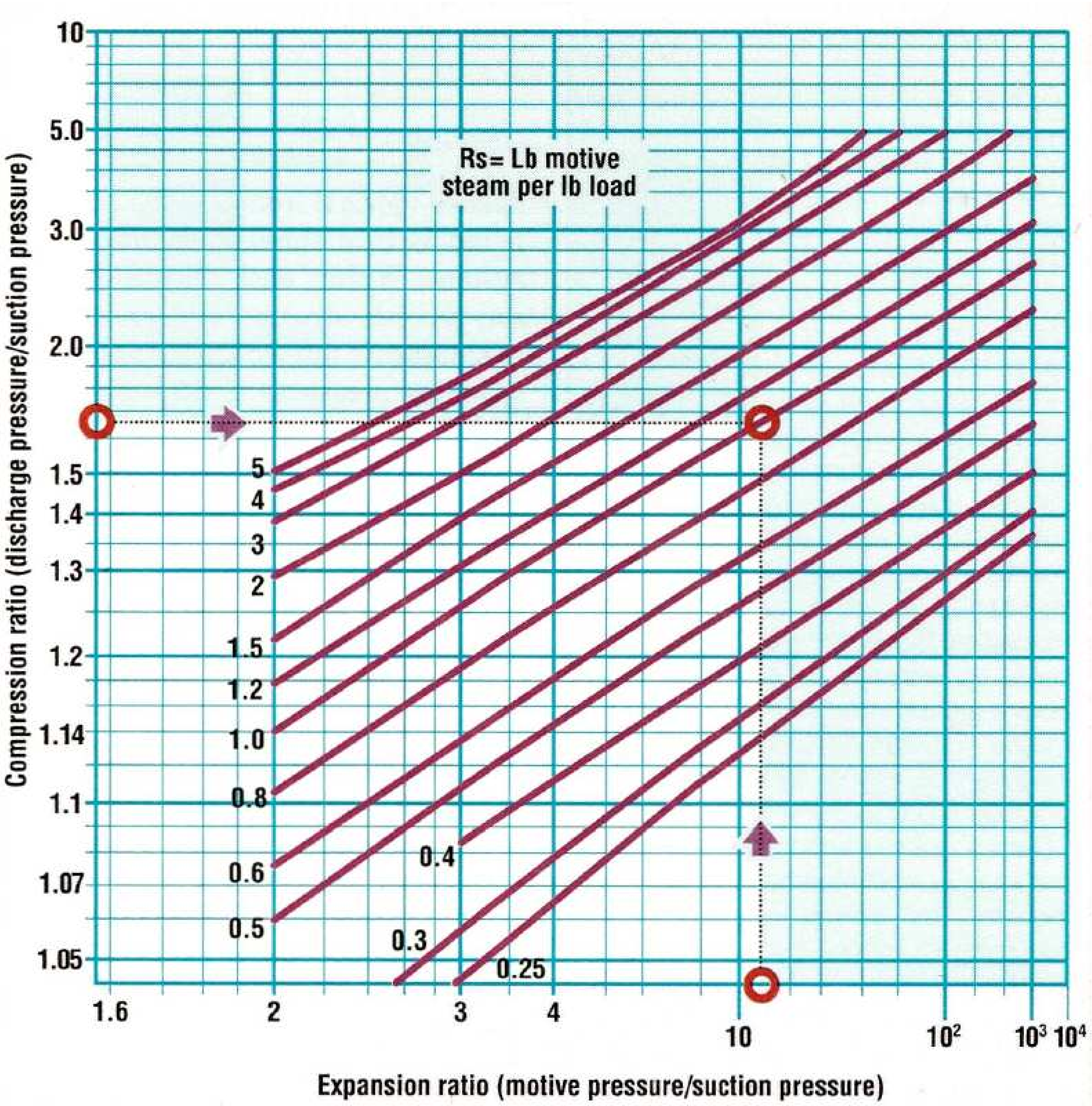
The steam thermocompression consists in using a steam jet ejector for recovery of low pressure steam (suction) by using high pressure steam (motive), obtaining medium pressure steam (discharge). It is an operation of interest to energy savings in processes.

The typical workflow for early assessment of a steam jet ejector is to get the required steam flow rate from charts available in manufacturers' catalogues (see HOKUTOMO, SCHUTTE & KOERTING and GEA) or in engineering textbooks (see PERRY *et al.*, 2008 and MINTON, 1986).

Some works, like EL-DESSOUKY *et al.* (2002) and MCGOVERN *et al.* (2012a, 2012b) , presented fundamental models from first thermodynamics principles, aiming to predict the irreversibilities and performance of real world ejectors. However predictive models like these can be much time-consuming and requires more information than that available during a prospective and early design stages.

In this context, Power (1994) proposed a graphical method that was constructed from performance information compiled from several commercially available ejectors. The chart used by Power is reproduced on Figure 2.3.

Figure 2.3: Plot of Compression ratio (CR) versus Expansion ratio (ER)



Source: POWER (1994)

In this work, models which correlate ratio of driving steam flow by suction steam flow with the ratios of compression and expansion in steam ejectors and their cost curves were analyzed and compared to each other, in order to select a simple model to implement.

References

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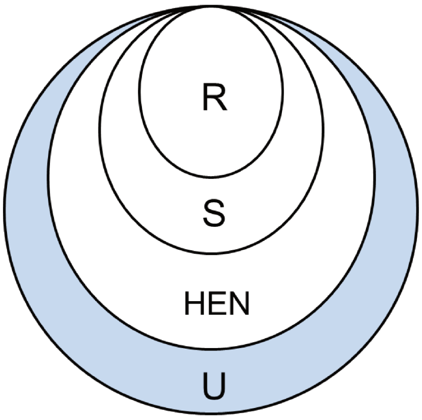
2.6 Utilities systems



2.6.1 Thermal insulation

Surfaces of equipment and pipes operating at non-room temperatures are subject to losses by thermal exchanges with the environment, both for heating and cooling operations. These losses have to be considered during the project of an industrial heat / cooling system and result in an increase of industrial plant energy consumption.

To minimize those thermal losses it is possible to increase insulation thickness. Several works have tackled the importance of a good insulation sizing and it is a typical energy saving rule. DOE-EERE (2009) shows some good practices regarding insulation sizing.

However industrial insulation can get very expensive if all good practice rules is followed and this issue is frequently neglected in early design stages.

Commercially available pre-insulated tubes (PIT) can reduce the overall costs associated with installation and application of industrial insulation (LOGSTOR, 2014).

Effects of wet insulation

Wet or moist insulation material can degrade insulation performance due to the increasing in insulation heat conductivity.

According to Pittsburgh Corning (1992), insulation thermal conductivity can increase by 30% with only 1% moisture (volumetric basis). A soaked insulation, with

20%(v/v) water content, can lead to a increase in heat losses up 300%, when compared with dry insulation (WILLIAMS, 2015).

These results, of course, are very dependent of the insulation material in analysis, and is specially worrying for fibrous insulation.

This work aims to assess the real feasibility of piping and equipment insulation and light on the losses components.

References

[1] DOE-EERE. **Improving Process Heating System Performance: A Sourcebook for Industry**, 2nd ed. 2009.

[2] LOGSTOR. **Pre-insulated pipes for industrial applications.** Available from: <https://www.logstor.com/media/1413/industry-general_en_p_in.pdf>. Access on 2014.

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Chapter 3

Methodology

3.1 General Methodology

Within the scope of the hierarchical design workflow, each hierarchical level requires go / no go decisions during design stage and/or diagnosis of existing processes. The present work intends to evaluate some technology options and the conditions that define designs and specifications to reduce energy consumption of chemical processes. This will be accomplished through the following steps:

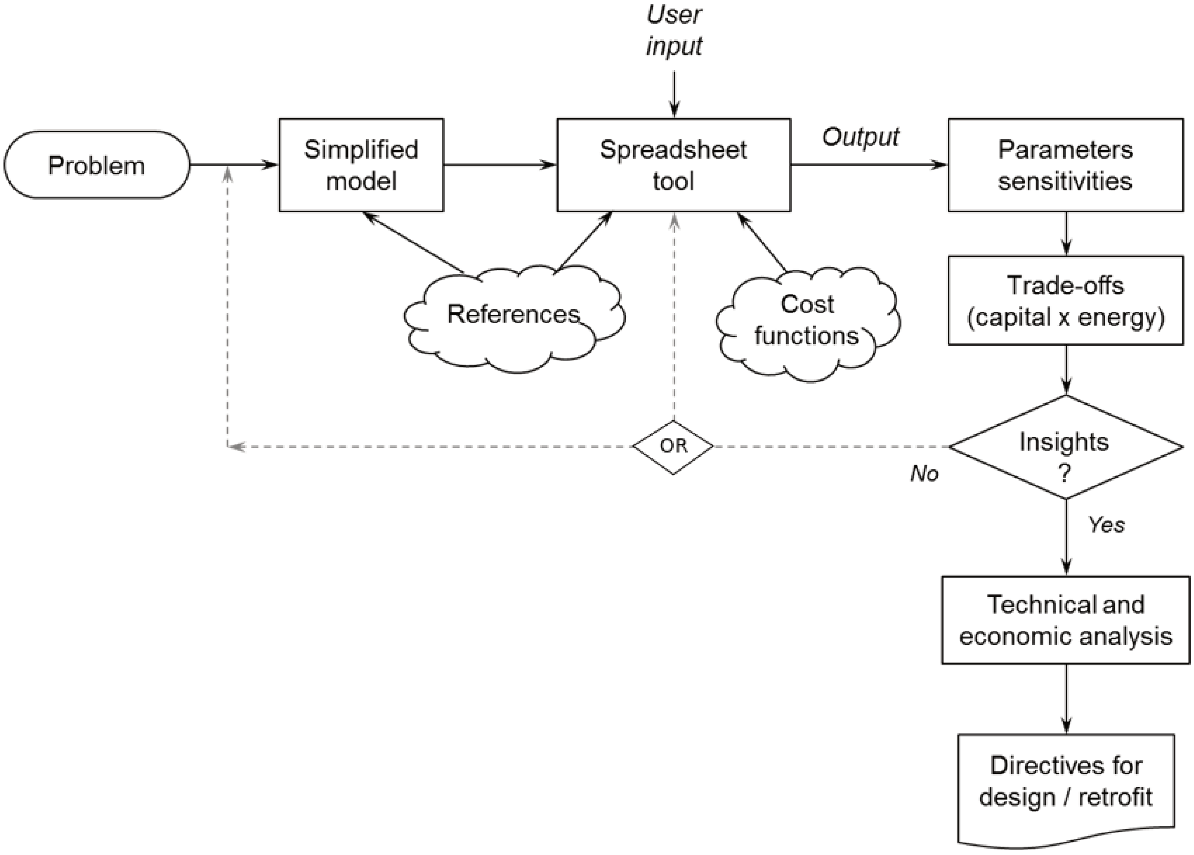
- Extensive, but not exhaustive, literature review of some selected elements of chemical processes on each layer of the “onion” model: reaction (chemical transformation processes), separation, heat transfer, fluid transport and allocation of utilities;
- Study of some systems and unit operations that constitute an industrial chemical process;
- Selection of the main factors that influence the energy efficiency of each system studied;
- Development of simplified models and computational tools for sizing and for the economic evaluation of equipment or systems.

The general methodology workflow consists on the following steps, sequential or simultaneous:

- From an objective problem, a simplified mathematical model is developed either from rigorous fundamental principles or from shortcut methods available from literature;
- Cost functions from the literature are used in the analysis in order to allow an economic assessment of the system.

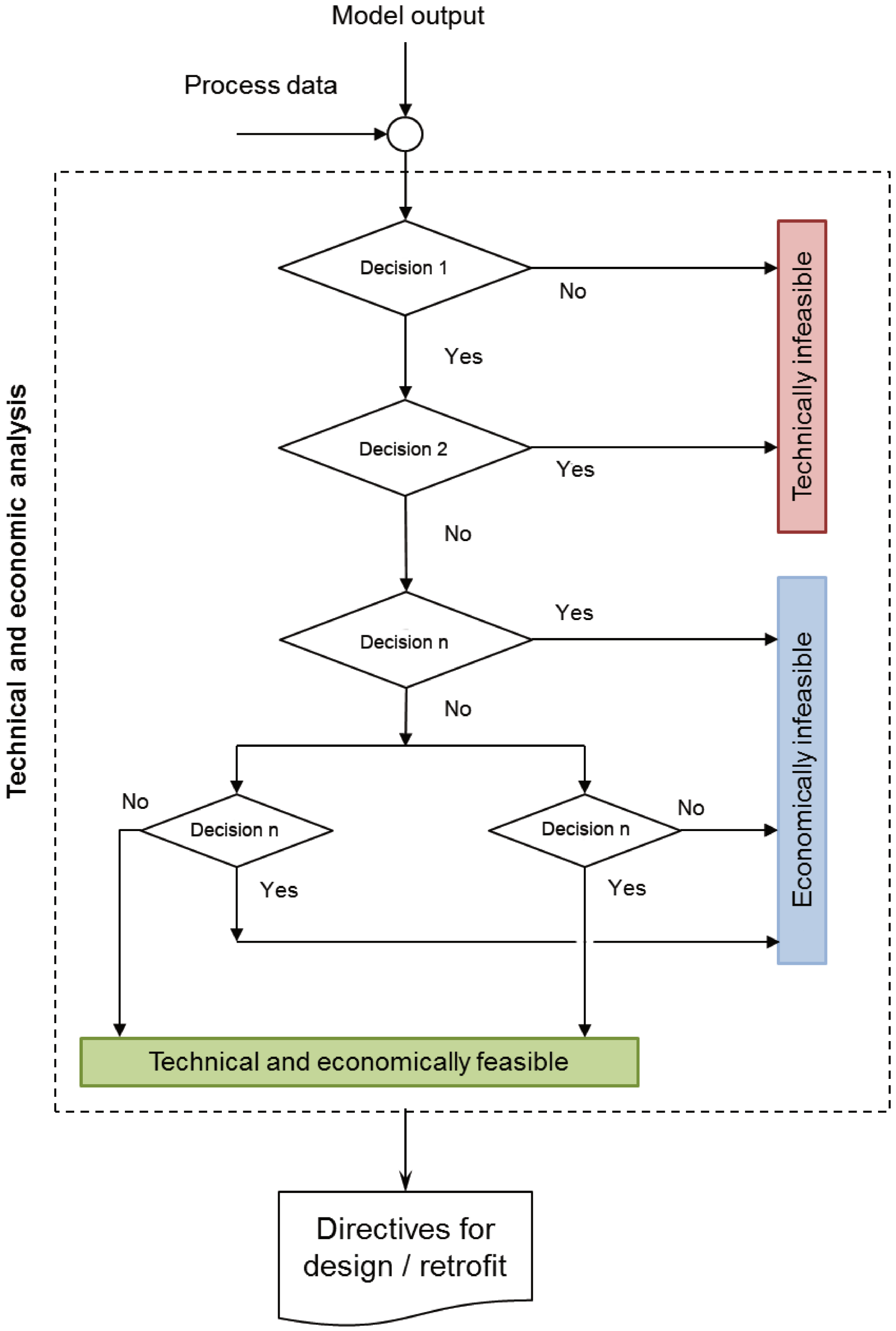
Figure 3.1 represents graphically the workflow of this general methodology.

Figure 3.1: General workflow of methodology



During a typical technico-economic analysis, a the results of physical and cost models undergo a sequence of yes / no decisions whether the proposed system is technically (physically attainable) and economically (financially attractive) feasible. Figure 3.2 shows a flowchart reproducing generally the workflow of inferring directives from the tools outputs (technical and economic analysis), based on the approach of KISS *et al.* (2011) and SHAH *et al.* (2012).

Figure 3.2: General flowchart of Technical and Economic feasibility analysis

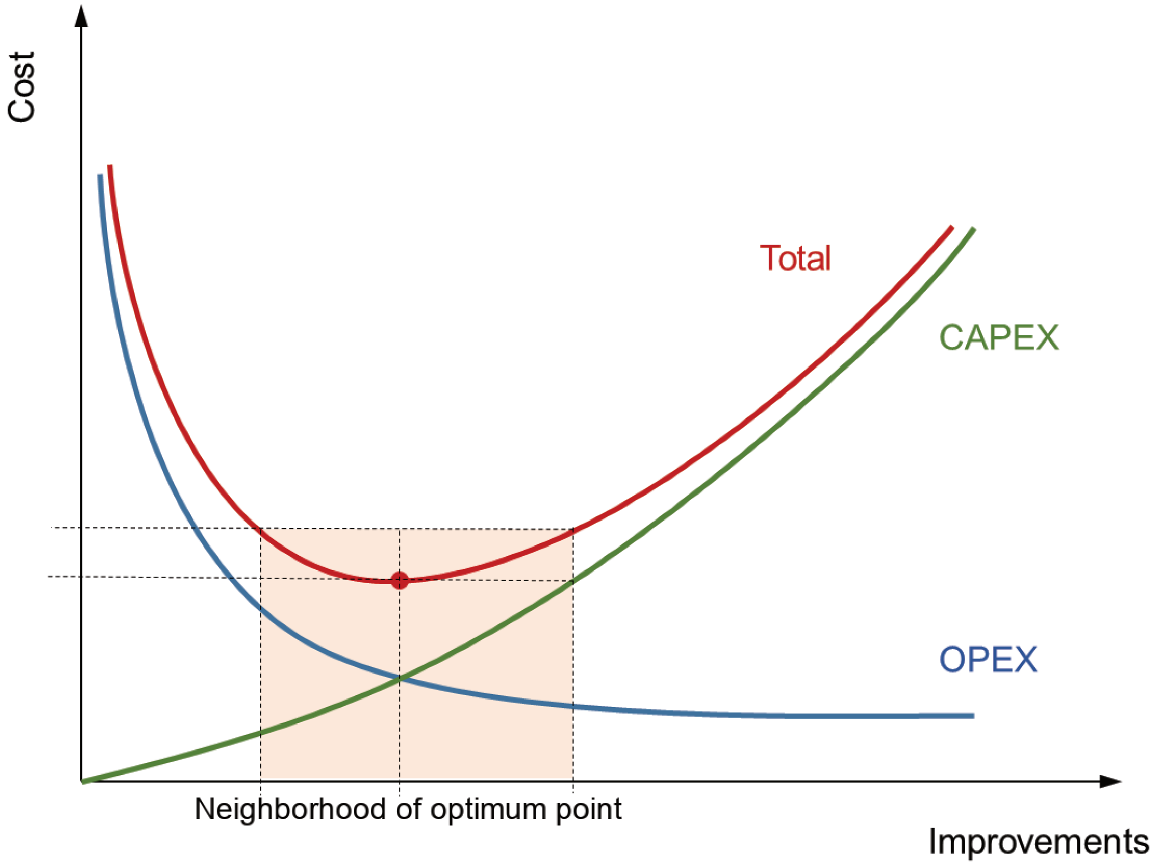


Most of the systems here addressed deals with a trade-off between capital expenditure ($CAPEX$) required for project execution and operational expenditures ($OPEX$) required to operate the process after project installation.

Figure 3.3 depicts a general Total Annualized Cost (TAC) curve which helps on the assessment of this trade-off.

It is important to note that mathematical optima must be taken with care, mainly on early stage approach studies, given the significant imprecision on cost estimations. For example, the shaded area in Figure 3.3 shows that there are no ways to discriminate between points lying in the close neighborhood of the optimum point.

Figure 3.3: General total cost composition and CAPEX x OPEX trade-off



Here (Figure 3.3), the horizontal axis depicts an increasing improvement effort, such as a larger diameter of a pipeline or a distillation column with more stages. This “effort” always comes with a price, so it is the annualized $CAPEX$ curve. For any project, it is expected that the additional cost of improvements bring savings, or in other words, to lower operating costs ($OPEX$).

Total cost approach allows the process engineer evaluate at an early stage of a project the best prospective alternative to engage on further detailing.

This approach will be applied for each studied system following the layers of the onion model, as listed in Table 3.1.

Table 3.1: Studied systems grouped by onion layers (and slice)

Layer	No.	Short description
R	1.1	Specific energy consumption in chemical processes
S	2.1	Heat pump assisted distillation
HEN	3.1	Heat Integration (single exchanger)
MTO	4.1	Pump and pipe system
	4.2	Steam turboexpansion
	4.3	Steam thermocompression
U	5.1	Thermal insulation

Cost curves

Several cost curves available in the literature were used for process equipment (pumps, exchangers, compressors, piping, etc.). These curves were obtained from established books on cost engineering, such as PETERS and TIMMERHAUS (1991, 2002), COUPER *et al.* (2012) and TOWLER and SINNOTT (2012).

All economic analyses were based on 2016. In cases where the available cost curve was based on previous years, these values were updated in time using the composite CEPCI[1] of 2016, as shown on Equation 3.1. The concept and definition of the CEPCI can be found in VATAVUK (2002).

$$\text{Cost}_{2016} = \text{Cost}_1 \cdot \frac{\text{CEPCI}_{2016}}{\text{CEPCI}_1} \tag{3.1}$$

where the index 2016 refers to the current year, and the index 1 refers to the year in which the cost curve used was based.

It is expected an imprecision on the CAPEX estimation on the order of $30\,\%$, that is in accordance with Order of Magnitude engineering studies during scope definition stage .

---

[1] The *Chemical Engineering Plant Cost Index* (CEPCI) is an established index used to adjust process plant construction costs from one time period to another. It is published monthly in the Chemical Engineering magazine since 1963.

Operational costs

On the analysis of economic trade-offs presented in this work, only the cost (or savings) with energy and maintenance of the equipment were considered. These costs are the most relevant ones that derive from the decision to go or not to go with the project under study on each topic, in comparison to an initial case.

Other costs, such as fixed costs (labor, facilities, etc.), non operational and administrative costs were not included in the analysis because it was assumed that these factors do not contribute to support the target decisions in this work, which basically aims to discriminate between technology options.

To support the calculation of operational costs, some assumptions were taken for all the studied cases and are shown in Table 3.2. Further specific assumptions can be found on each section.

Table 3.2: Base values used in this work for accounting operational costs

Annual operational time (OH)	$8600\,\mathrm{h/year}$
Power cost (C_{power})	$\$0.15\,/\mathrm{kWh}$
Steam cost (C_{steam})	$\$30\,/\mathrm{t}$
Maintenance cost (C_{maint})	$3\,\%$ of CAPEX $/\mathrm{year}$

For the total annualized cost, 10 year operating time was assumed, so the TAC is calculated by Equation 3.2.

$$TAC = \frac{\text{Investment cost}}{10} + \text{Operating cost} \tag{3.2}$$

The simple payback can be written as:

$$PB = \frac{\text{Investment cost}}{\text{Savings}} \tag{3.3}$$

In some cases, the savings must not be compared against an absolute investment cost, but against a incremental investment cost, being thus written as:

$$PB = \frac{(\text{Investment cost}_{\text{alternative}} - \text{Investment cost}_{\text{base}})}{\text{Savings}} \tag{3.4}$$

Models

Each simplified model is described in its own section in this chapter. It is also available a process template, descriptive equation and the models that were used for cost evaluation.

It is not the objective of this work to delve into the first principles, phenomenological and constitutive models that describe the phenomena in each of the topics. In other words, mathematical models that are well defined in literature have been left out of the Methodology chapter.

Only the equations necessary for the development of sensitivity analyses and those that are required to connect the physical and cost models will be described.

Tools

All spreadsheets were developed using Microsoft Excel® over which all mathematical models described in this section were implemented, as well as the parameters variation automation to build the sensibilities. The mathematical models and cost curves were coded as VBA functions and grouped as shared libraries, allowing easy integration among other spreadsheets.

The developed tools and models are not intended to be used as predictive design tools. The simplifying assumptions adopted may degrade the accuracy of the results for a single design condition, but are still sufficiently accurate for the comparative assessment on sensitivity analyses.

The models are intended to give “optimistic” results, so minimizing the risk of some result suggesting to discard a potential good idea at an early stage.

All the tools developed on the realm of this work are freely available with the author.

References

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3.2 Reaction

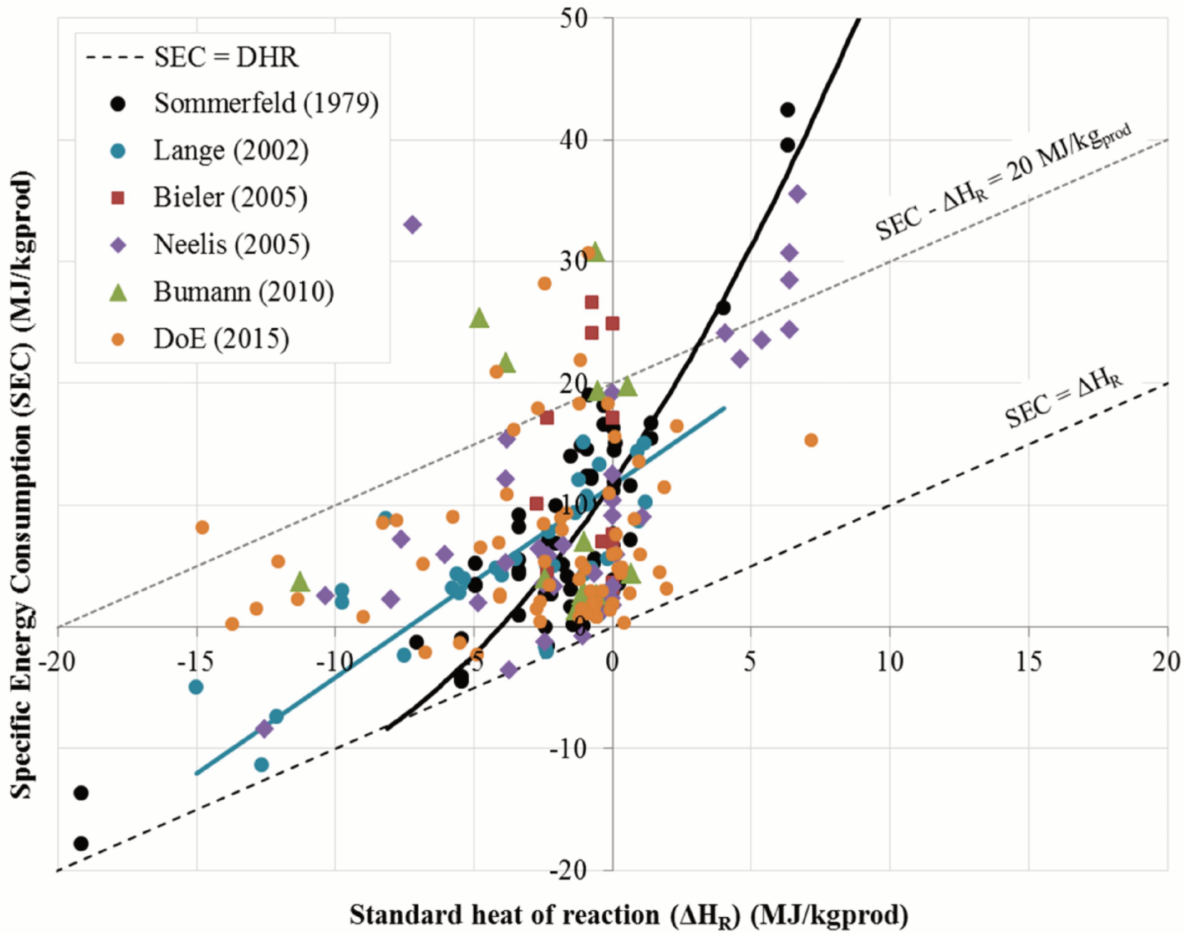
3.2.1 Specific energy consumption in chemical processes

This work gathered all data informed by the authors mentioned in the literature review section and proposed a simple conciliation for SEC as a function of $\Delta H^\circ_\mathrm{R}$ points, where $\Delta H^\circ_\mathrm{R}$ is the standard enthalpy of reaction at 25°C, defined as the difference between enthalpy of formation of product of interest and enthalpy of formation of the raw materials (reactants), as shown on Equation 3.5.

$$\Delta H^\circ_\mathrm{R} = \frac{1}{\nu_\mathrm{prod} M_\mathrm{prod}} \sum_i \nu_i \Delta h^\circ_{\mathrm{f},i} \tag{3.5}$$

A summary of the collected data points, along with their sources, and the nature of the products are listed in Table 3.3 and illustrated in Figure 3.4. From the cloud of points it's clear that, although scattered, there is a visible relation between $\Delta H^\circ_\mathrm{R}$ and SEC. The correlation of Sommerfeld and a fitting to Lange's data are also shown.

Figure 3.4: Specific Energy Consumption versus Standard Enthalpy of reaction for data points listed in Table A.1, with correlation (Sommerfeld) and linear fitting to data (Lange)



Some of the data sets show distinct values for the same products manufactured by the same pathways. These values were kept in the analysis because they reflect the reality of the variability due to different manufacturers and different pathways. The whole data set compiled in this work is tabulated on Table A.1.

Table 3.3: Data sources, thermodynamic function and type of product analyzed

Datasets sources	**Number of points**	**Thermodynamic function**	**Range of ΔX_R (MJ/kg)**	**Range of SEC (MJ/kg)**	**Type of product**
Sommerfeld and White (1979)	66	ΔH_R	-19.2 – 6.3	-17.8 – 42.4	Petrochemical and base chemicals
Lange (2001)	35	ΔH_R	-15.0 – 1.2	-11.3 – 15.2	Petrochemical and base chemicals
Bieler *et al.* (2005)	15	ΔH_R	-2.7 – 0	2 – 26.6	Chemical Specialties
Neelis *et al.* (2005)	40	ΔH_R	-12.5 – 6.7	-8.4 – 45.6	Petrochemical and base chemicals
Bumann *et al.* (2010)	14	ΔH_R	-11.3 – 0.67	1.4 – 30.8	Solvents
US DoE (2015)	67	ΔG_R	-14.8 – 7.2	-5.8 – 30.7	Petrochemical and base chemicals
Total	**238**				

Note: $\Delta X_\mathrm{R} = \Delta H_\mathrm{R}$ or ΔG_R

Analyzing Figure 3.4, it's possible to observe:

- Sommerfeld and White's (1979) correlation doesn't predict well the SEC for exothermic reactions with $\Delta H^\circ_\mathrm{R}$ < -5 MJ/kg of product;
- Lange's (2002) curve misses the SEC for endothermic processes;
- Bieler *et al.* (2005), Neelis *et al.* (2005), Bumann *et al.* (2010) and DoE (2015) only presented the data for SEC and $\Delta H^\circ_\mathrm{R}$; no correlations were proposed.

This work proposes a new correlation between SEC and $\Delta H^\circ_\mathrm{R}$ conciliating some works published so far in this theme.

List of symbols

Symbol	**Description**	**Unit**
SEC	Specific Energy Consumption (reported)	$\mathrm{kcal/kg}$ of product
SEC'	Specific Energy Consumption (estimated)	$\mathrm{kcal/kg}$ of product
σ	Standard deviation of reported SEC	$\mathrm{kcal/kg}$ of product
ν_i	Stoichiometric number of substance i	-
$\Delta h^\circ_\mathrm{f,i}$	Standard Enthalpy of formation of substance i	$\mathrm{kcal/mol}$ of i
$\Delta H^\circ_\mathrm{R}$	Standard Enthalpy of reaction	$\mathrm{kcal/kg}$ of product
$\Delta G^\circ_\mathrm{R}$	Standard Gibbs energy change due to reaction	$\mathrm{kcal/kg}$ of product
M_prod	Molecular mass of product of interest	$\mathrm{kg/kmol}$ of product

References

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3.3 Separation operations

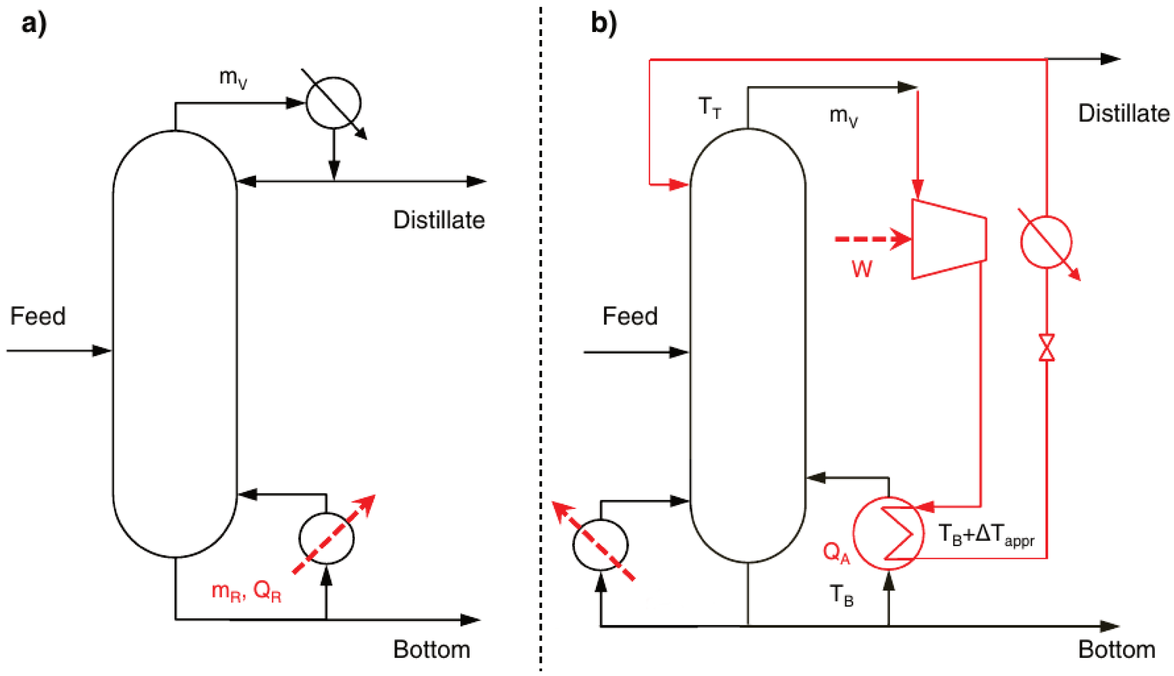
3.3.1 Heat pump assisted distillation

In a heat pump assisted distillation column, a portion of the heat that would be discarded on tower's condenser is "pumped" back to reboiler, making use of a refrigeration cycle.

In this work, we will focus on heat pumps based on vapor compression cycle, using the own top column vapor (open cycle) as the working fluid into a mechanical compressor. This set-up is often called a MVC (mechanical vapour compression) distillation column.

Figure 3.5 shows simplified diagrams of conventional distillation column (a) and a heat pump assisted distillation column (b). The main parameters of the CAPEX x OPEX trade-off are highlighted in red in the figure.

Figure 3.5: Simplified diagram comparing conventional distillation column (a) and a heat pump assisted distillation column (b)



Trade-off

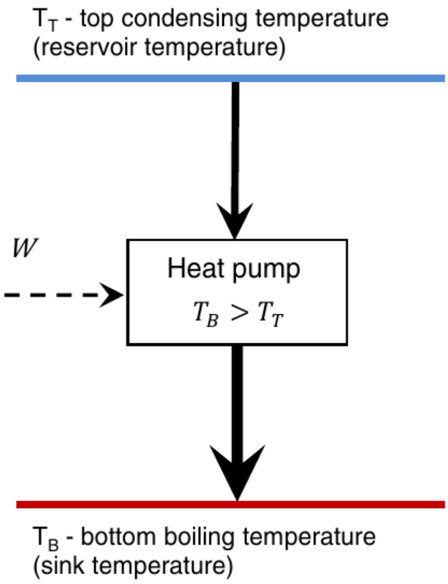
As shown on Figure 3.5, the feasibility of such alternative relies on the trade-off between the cost of the steam consumed in the column's reboiler (conventional distillation) and the cost of the electricity used to run the mechanical compressor (MVC distillation). Surely such feasibility is strongly dependent on the relative costs between electrical and thermal energies, but also on the overall system efficiency and the required temperature "lift" to be driven by the heat pump between column's top and bottom.

As in any heat pump, we can define for this system a Coefficient of Performance (COP) that express the heat that can be "pumped" by each unit of work consumed.

In this case, the useful heat supplied by the heat pump is the sum of the heat removed from the source (heat of condensing of the top product - Q_{top}) and the work applied to the compressor (W), as outlined on Figure 3.6 and Equation 3.6.

$$COP = \frac{Q_{\text{top}} + W}{W} \tag{3.6}$$

Figure 3.6: Simplified diagram of a generalized heat pump



The maximum (unattainable) thermodynamic COP can be derived from a reverse-working Carnot's engine, as shown on Equation 3.7.

$$COP_{\text{max}} = \frac{T_{\text{bot}} + \Delta T_{\text{appro}}}{T_{\text{bot}} + \Delta T_{\text{appro}} - T_{\text{top}}} \tag{3.7}$$

The overall heat pump efficiency (η_{over}) takes into account all non-idealities present in the system. It can be expressed as Equation 3.8.

$$\eta_{\text{over}} = \frac{COP}{COP_{\text{max}}} \tag{3.8}$$

According to MESZAROS and FONYÓ (1986), typical values for real COP range from 5 - 7.

Assumptions

In order to improve the simplicity of the sensitivity analyses, only costs with steam (in conventional distillation) and electricity (in MVC distillation) were considered. Other savings that are ultimately brought by the heat pump assisted distillation, such as reduced cooling water consumption, or other costs, such as increased maintenance costs, were not considered.

It is expected that those simplifications on the cost models will be diluted among the general imprecision of $CAPEX$ estimates of the order of ± 30 %.

Further general assumptions:

- Constant condensing temperature;
- Constant boiling temperature;
- Top product vapor behaves as an ideal gas;
- Default polytropic efficiency = 0.7;
- Temperature increase due to superheating after compression was neglected;
- For calculations involving $\Delta T_{\text{b-t}}$, $T_{\text{bot}} = 105\,°\text{C}$ was assumed at bottom;
- The total heat ($Q_{\text{top}} + W$) lifted to reboiler temperature is greater than or equal to required reboiler duty;
- The excess heat added to the system is removed by a trim cooler;
- The capital expenditure (CAPEX) considered in Equation 3.15 accounts only for the incremental installed cost of vapour compression apparatus.

Physical model

Required work (polytropic compression):

$$W = \eta_p W_p = \eta_p \frac{\mathrm{nR}T_{\text{top}}}{n-1}\left[\left(\frac{P_{\text{out}}}{P_{\text{top}}}\right)^{\frac{n-1}{n}} - 1\right] \tag{3.9}$$

where

$$n = \frac{\eta_p \gamma}{1 + \eta_p \gamma - \gamma}$$

Required temperature at compressor outlet:

$$T_{\text{out}} = T_{\text{bot}} + \Delta T_{\text{appro}} + \Delta T_{\text{sheat}} = T_{\text{top}}\left(\frac{P_{\text{out}}}{P_{\text{top}}}\right)^{\frac{n-1}{n}} \tag{3.10}$$

Cost model

The savings of operating a heat pump assisted distillation column instead a conventional one can be reasonably approximated to:

$$\text{Savings} = OPEX_1 - OPEX_2 = OH\left(\dot{m}_{\text{steam}} \cdot C_{\text{steam}} - W \cdot C_{\text{power}}\right) \tag{3.11}$$

In order to compare the costs of different energy sources (steam and power), it is necessary to define a relation between them, as shown on Equation 3.12.

$$\frac{\text{\$ EE}}{\text{\$ Steam}} = \frac{C_{\text{power}}\,[\$/\mathrm{kWh}]}{\dfrac{C_{\text{steam}}\,[\$/\mathrm{t}]}{\lambda_{\text{steam}}\,[\mathrm{Mcal/t}]}\dfrac{0.8604\,[\mathrm{Mcal}]}{1\,[\mathrm{kWh}]}} \tag{3.12}$$

The simple payback (PB) time can be written as:

$$PB = \frac{CAPEX}{OPEX_1 - OPEX_2} \tag{3.13}$$

$$= \frac{CAPEX}{OH(\dot{m}_{\text{steam}} \cdot C_{\text{steam}} - W \cdot C_{\text{power}})} \tag{3.14}$$

$$= \frac{CAPEX}{OH \cdot \dot{m}_{\text{steam}} \cdot C_{\text{steam}}\left(1 - \dfrac{\text{\$ EE}}{\text{\$ Steam}}\dfrac{1}{COP}\right)} \tag{3.15}$$

The Equation 3.15 can be rewritten to

$$COP = \left(\frac{1}{1 - \dfrac{CAPEX}{PB \cdot OPEX_1}} \right) \frac{\text{\$ EE}}{\text{\$ Steam}} \tag{3.16}$$

This equation is useful to get the break-even COP to get a given payback time.

A study of sensitivity in respect to process parameters was prepared in order to find ranges of technical and economic feasibility of distillation process coupled with the heat pump.

The combined use of the physical and cost models was basis to develop the sensitivity analyses shown on section 4.3.1.

References

[1] MESZAROS, I.; FONYÓ, Z. **Design strategy for heat pump assisted distillation system.** *Heat Recovery Systems.* Vol. 6, No. 6, pp. 469-476, 1986.

List of symbols

Symbol	Description	Unit
COP	Coefficient of Performance	$\mathrm{kW_t/kW_e}$
W	Compressor work	W
Q_{bot}	Reboiler heat duty	W
Q_{top}	Condenser heat duty	W
$\dot{m}_{\text{steam}}$	Reboiler steam mass flow rate	t/h
λ_{steam}	Enthalpy of vaporization of steam	kcal/kg
η_{over}	Overall efficiency	-
T_{bot}	Bottom temperature	°C
T_{top}	Top temperature	°C
ΔT_{appr}	Minimum temperature approach in reboiler and condenser	°C
$\Delta T_{\text{b-t}}$	Temperature difference between bottom and top	°C
T_{out}	Compressor outlet temperature	°C
P_{top}	Top pressure	bar a
P_{out}	Compressor outlet pressure	bara
$OPEX_1$	Operational cost of conventional distillation	\$/y
$OPEX_2$	Operational cost of MVC distillation	\$/y
$CAPEX$	Incremental capital expenditure	\$
OH	Annual operating time	h/y
Cp	Specific heat at constant pressure	kcal/ kg °C
Cv	Specific heat at constant volume	kcal/ kg °C
m_V	Top vapour mass flow	kg/h
U	Overall Heat Transfer Coefficient	kcal/h °C m^2
ΔT_{sheat}	Temperature increase due to superheating	°C
γ	Vapour Cp/Cv	-
η_p	Polytropic compression efficiency	-

3.4 Heat transfer operations

3.4.1 Thermal Integration

In energy integration projects, usually the heat exchanger network designed to reach minimum energy consumption may present itself very complex and uneconomical.

A simplified model was developed, aiming to prospect a relevant integration with low investment.

This model assumes that a pair of hot and cold streams has been identified as potential for thermal integration.

Figure 3.7 shows a simplified diagram of the 2 streams demanding heating and cooling, respectively, through utilities.

Once a list of pairs of streams has been identified, the developed tool can be used to rank the most promising pair(s) in terms of technical-economic feasibility.

This is intended to be a tool for preliminary prospection, using little information to help on the screening of multiple integration ideas.

Figure 3.8 shows a simplified diagram of a heat integration set-up, between streams shown on the previous figure.

Figure 3.7: Simplified diagram of the heating and cooling processes met by utilities

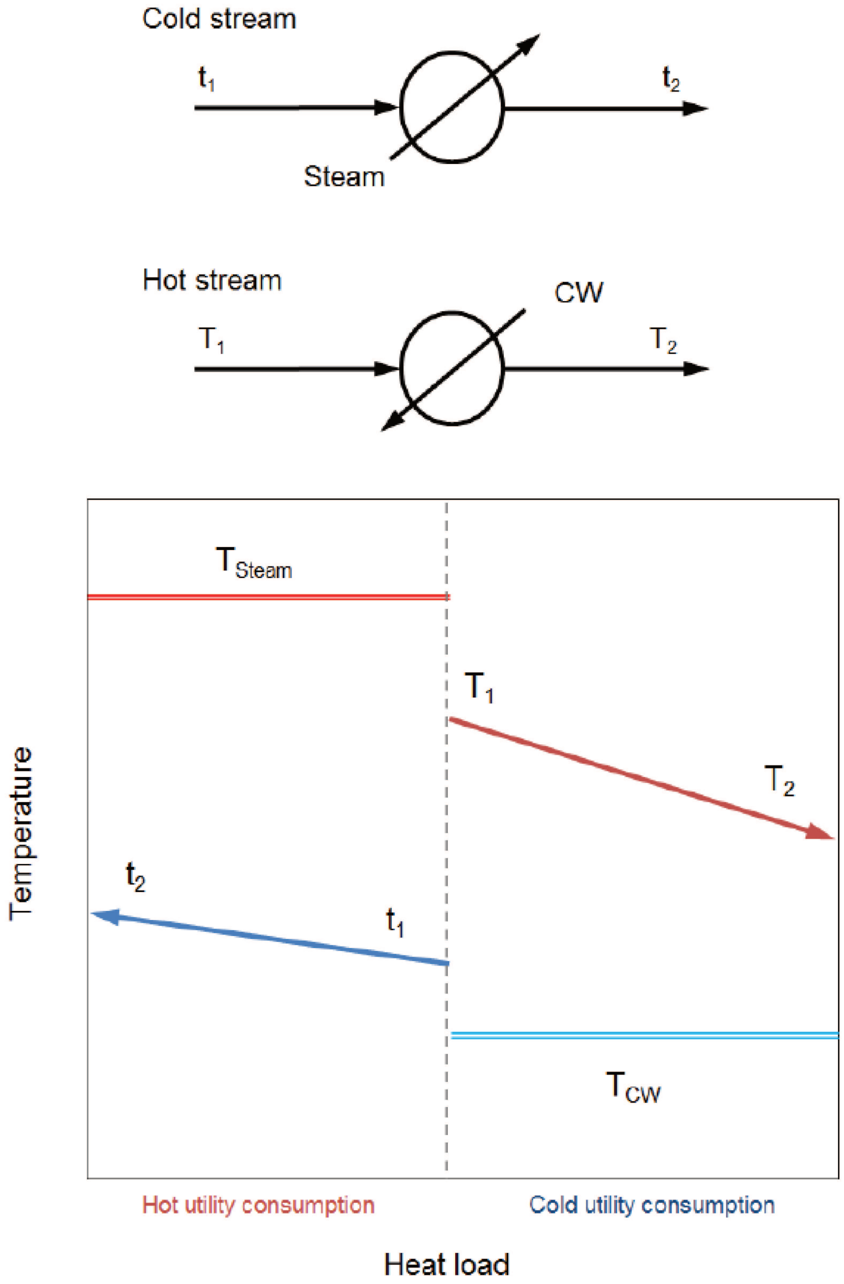
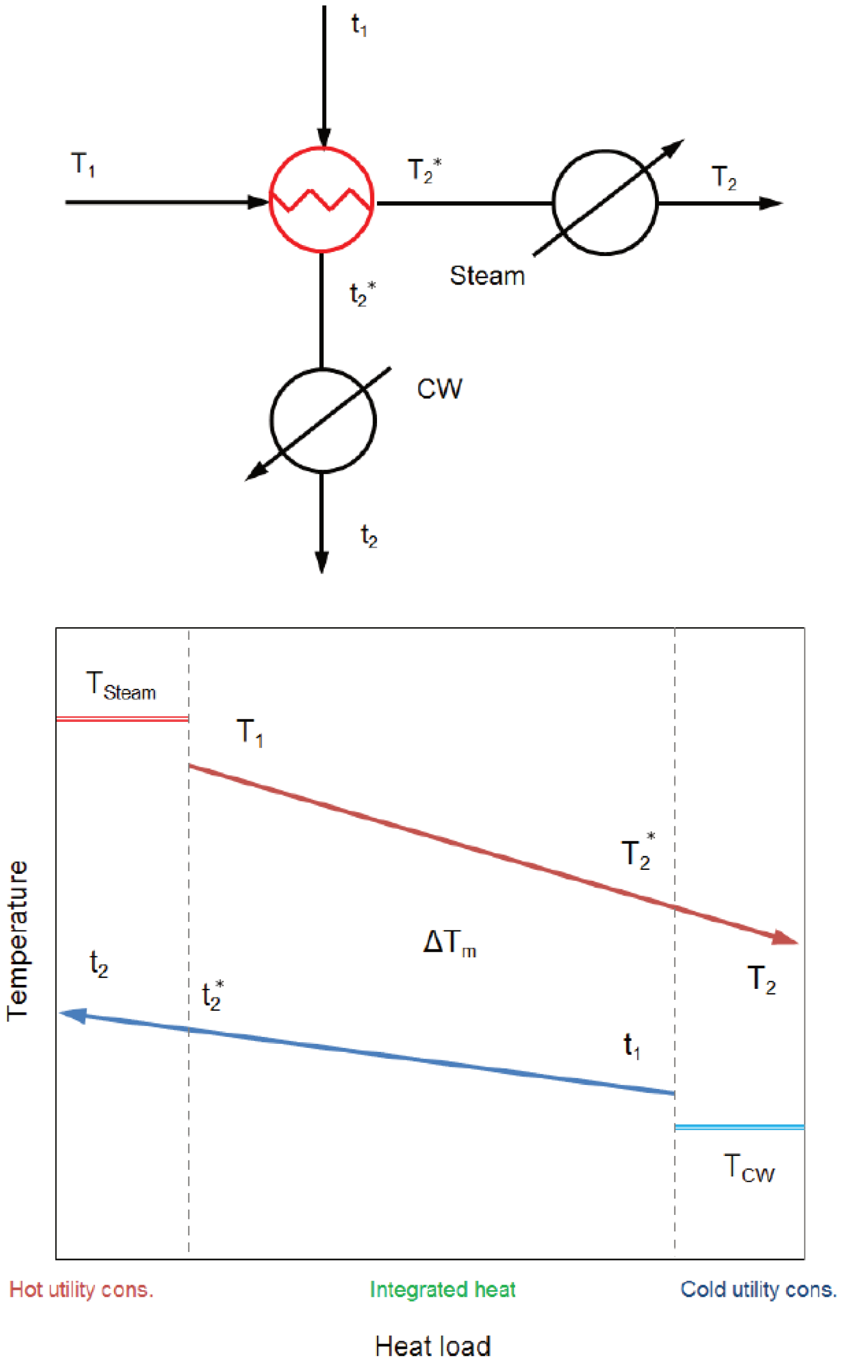


Figure 3.8: Simplified diagram of the prospective heat integration



Trade-off

The potential economic feasibility of this set-up relies on cost of installing a additional heat integration exchanger versus the savings in hot and cold utilities when the whole heating and cooling demands are met by utilities alone.

Assumptions

In order to keep the model as simple as possible, some assumptions were taken:

- Single pass counter-current heat exchanger;
- Sensible heat heating and cooling occurs at constant c_P;
- Pure phase changing processes can be represented by choosing an equivalent $c_P \Delta T$.

Physical model

General heat exchange equation:

$$q = UA \cdot \Delta T_{\mathrm{M}} = \dot{m}_S \lambda_S \tag{3.17}$$

where

$$T_{\mathrm{M}} = \begin{cases} LMDT = \dfrac{(T_1 - t_2) - (T_2 - t_1)}{\ln \dfrac{T_1 - t_2}{T_2 - t_1}}, \ \dfrac{T_1 - t_2}{T_2 - t_1} \neq 1 \\ T_1 - t_2, \ \dfrac{T_1 - t_2}{T_2 - t_1} = 1 \end{cases}$$

Cost model

The purchased cost of heat exchanger is assumed to be only function of area and material.

$$C_E = f(A, \text{material}) = a \cdot A^{\alpha} \ \text{[k\$]}$$

The saved steam cost is given by:

$$\text{Savings} = \dot{m}_S \cdot C_{\text{steam}} \cdot OH \ \text{[k\$/y]}$$

$$PB = \frac{F_I \cdot C_E}{\text{Savings}} = F_I \cdot \frac{a \cdot A^{\alpha} \lambda_S}{UA \cdot \Delta T_{\mathrm{M}} \cdot C_{\text{steam}} \cdot OH} \ \text{[y]} \tag{3.18}$$

$$PB = \beta \frac{1}{U \cdot \Delta T_{\mathrm{M}}}, \text{ where } \beta = \frac{F_I \cdot a \cdot \lambda_S}{C_{\text{steam}} \cdot OH} A^{\alpha - 1} \tag{3.19}$$

$$\frac{1}{U \cdot \Delta T_{\text{M}}} = \frac{PB}{\beta} = \frac{C_{\text{steam}} \cdot OH}{a \cdot \lambda_S} A^{1-\alpha} \tag{3.20}$$

Using this model, a sensitivity analysis has been performed in order to obtain fields of technical and economic feasibility of implementing of individual heat exchanger for thermal integration and thus help to identify potential projects.

List of symbols

Symbol	Description	Unit
U	Overall heat exchange coefficient	$\mathrm{kcal/h/m^2/°C}$
Q	Exchanger heat duty	kcal/h
C_{steam}	Unitary steam cost	\$/t
Q^*	Integrated heat duty	kcal/h
A	Exchanger heat duty	$\mathrm{m^2}$
T_1	Hot side inlet temperature	°C
T_2	Hot side outlet temperature	°C
t_1	Cold side inlet temperature	°C
t_2	Cold side outlet temperature	°C
ΔT_{M}	Mean temperature difference	°C
$\dot{m}_{\text{steam}}$	Reboiler steam mass flow rate	t/h
λ_{steam}	Enthalpy of vaporization of steam	kcal/kg
OH	Annual operating time	h/y
F_I	Installation factor	-
CW	Cooling water	-

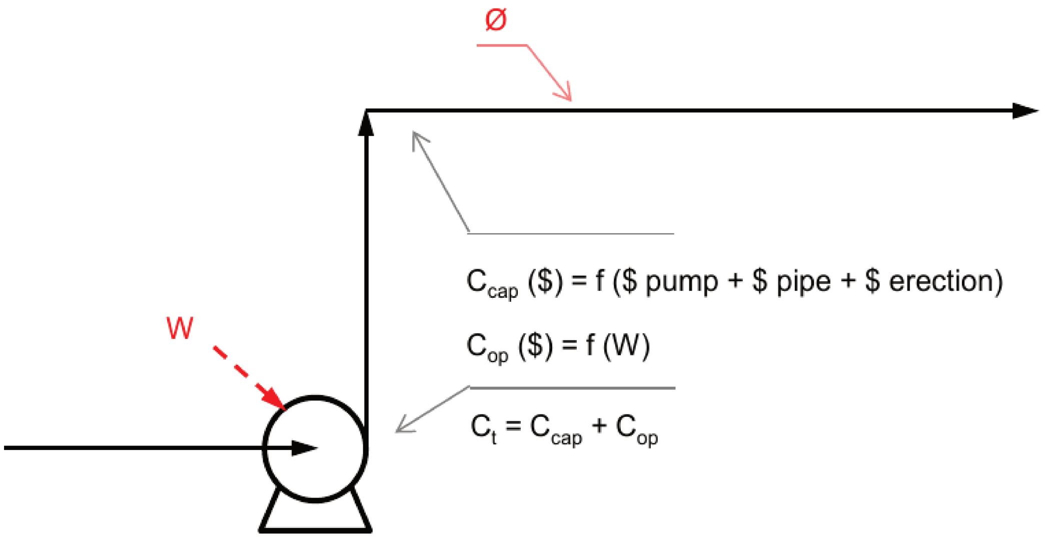
3.5 Momentum transfer operations

3.5.1 Pumping systems

Figure 3.9 shows a simplified schematic of a pumping system. System total costs comprise of installed cost of pump + piping and operational cost.

The main parameters for CAPEX vs OPEX trade-off are highlighted in red on the diagram.

Figure 3.9: Simplified schematics of a pumping system



Trade-off

The trade-off in this system is based on the economic feasibility of designing a piping system with larger diameter (more expensive in investment) in order to minimize the operating costs in pumping energy consumption.

Assumptions

The developed tool utilizes models, with the following assumptions:

- Installation costs consider only a pump and straight pipes;
- Incompressible flow;
- Fittings and accessories must be considered as equivalent length of straight pipe (see CRANE, 2010 for reference).

Model

The required pumping power is given by Equation 3.21

$$W_{\text{pump}} = \frac{Q \cdot \Delta P}{\eta} \tag{3.21}$$

where

$$\Delta P = \Delta P_{\text{friction}} + \Delta P_{\text{head}} \tag{3.22}$$

The pressure drop due to friction $\Delta P_{\text{friction}}$ is a function of the roughness of pipe material, fluid properties and flow rate.

$$\Delta P_{\text{friction}} = f(Re, D, Q, \varepsilon) \tag{3.23}$$

The developed tool utilizes this models and fluid properties to calculate the the pump's power consumption in function of the given flow rate. Some sensitivity analyses were performed in order to identify guidelines on the identified trade-off.

List of symbols

Symbol	Description	Unit
W_{pump}	Pump power	W
ΔP	Pumping total head	Pa
$\Delta P_{\text{friction}}$	Head loss due to friction	Pa
ΔP_{head}	Static head	Pa
η	Pump efficiency	$-$
Q	Total volumetric flow	$\mathrm{m^3/s}$
ε	Pipe material roughness	mm
D_{opt}	Optimum pipe diameter	in
v_{opt}	Optimum economical velocity	$\mathrm{m/s}$
Re	Reynolds number	-

References

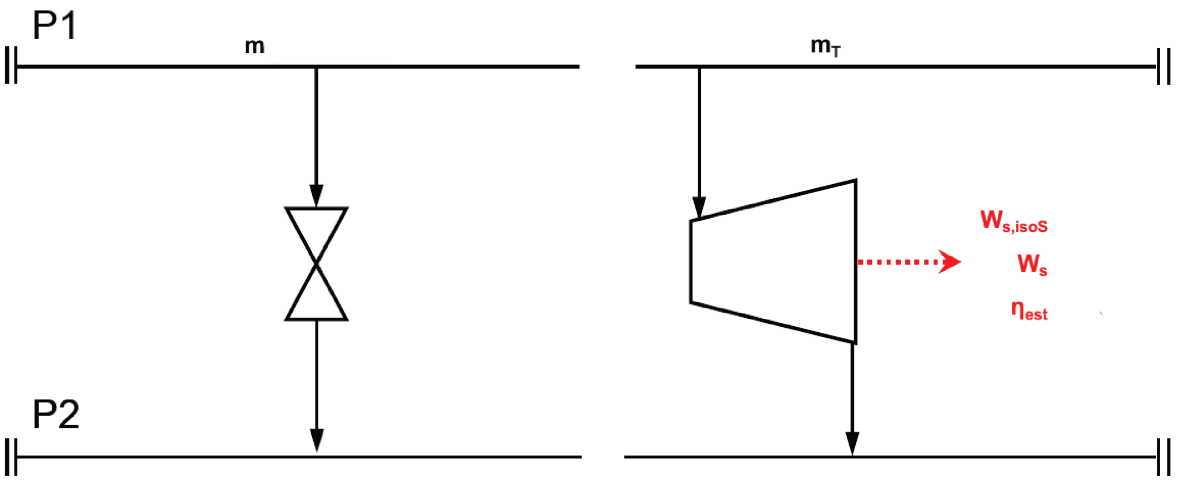
[1] CRANE. **Flow of Fluids - Through Valve, Fittings and Pipes** – Technical Paper No. 410. Crane Co., 2010.

3.5.2 Steam turboexpansion

This study provides a quick cost and performance evaluation of performing steam pressure reduction using a turboexpansion system instead of a throttle valve.

Figure 3.10 shows a schematic diagram of a turboexpander set-up, in comparison to a throttle valve. The two headers represent two levels of steam pressure ($P_1 > P_2$).

Figure 3.10: Simple schematic of a steam network with two pressure levels



a) *Throttle Valve*

b) *Turboexpander*

Trade-off

The economic feasibility of this set-up relies on the installation cost of a steam turbine versus shaft work generated from steam expansion. This feasibility is strongly dependent on the total amount of energy recoverable and the overall efficiency of the turbogenerator set-up.

Assumptions

In order to keep the analysis as simple as possible, the following assumptions were adopted:

- Expansion at valve is considered isenthalpic;
- For turbine, isentropic efficiency curve in respect to rated power was assumed (see Figure 3.11);

- Inlet steam sufficiently superheated to not occur condensation during expansion;
- Costs of purchase and installation of throttle valve are assumed negligible front to turbine costs;
- Turbine efficiency and cost are estimated on each rated power;
- Investment costs include turbogenerator set and auxiliary installation costs. It is expected the analysis performed still valid for turbine-driven machine sets;
- Annual maintenance cost is relative to equipment cost;
- Turbine efficiency curve is interpolated up to 3 MW.

Model

The potential work recovery derives from the work lost due to the unresisted expansion at throttle valve. The resisted expansion nature of the steam turboexpansion allows less entropy generation and, consequently, use of the a net shaft work.

The isentropic shaft work ($W_{\mathrm{S,isoS}}$) that would be ideally generated from steam expansion in the turboexpander is expressed by Equation 3.24.

$$W_{\mathrm{S,isoS}} = \dot{m}_{\mathrm{T}} \left(h_1 - h_{2,S}\right) \tag{3.24}$$

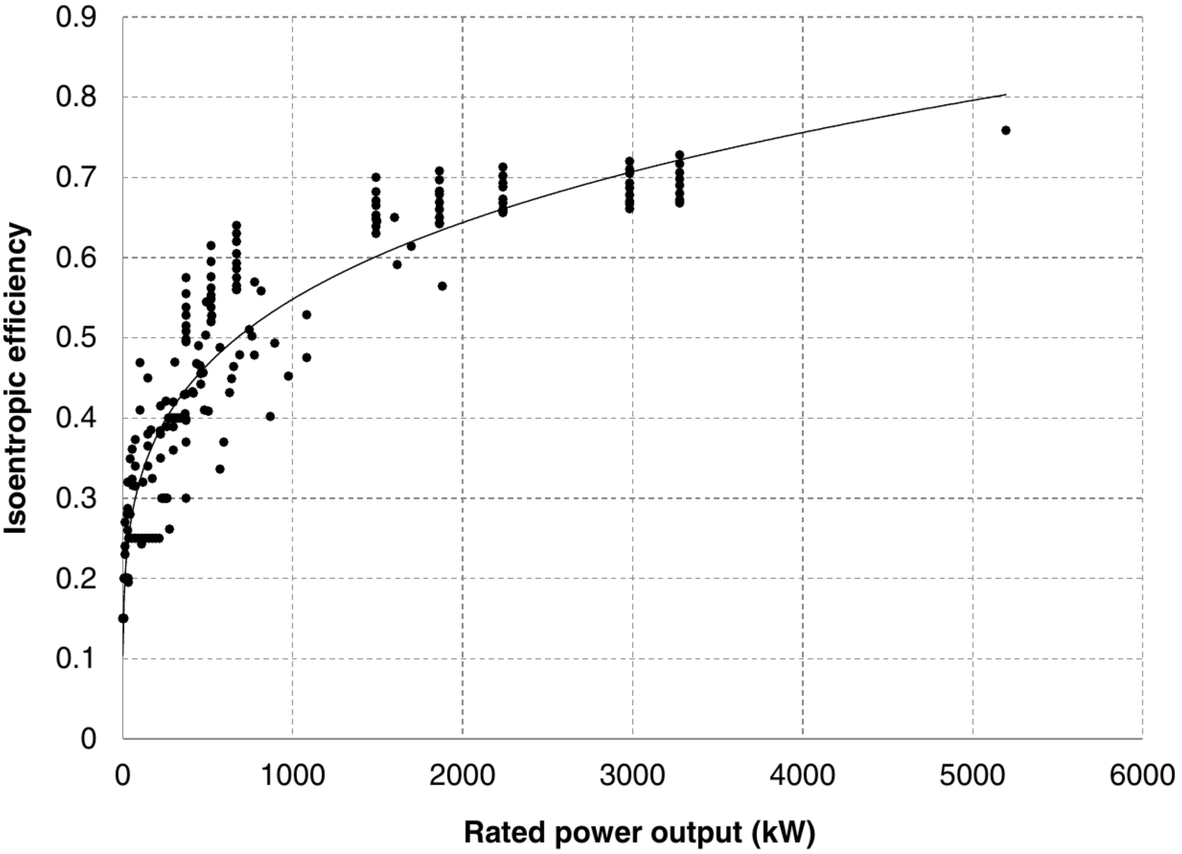
For specific enthalpy calculations, the IAPWS/97 formulation was used (WAGNER *et al.*, 1997) as implemented in VBA library Water97 (version 1.3) (SPANG, 2002).

The real shaft work (W_{S}) is a fraction of $W_{\mathrm{S,isoS}}$, given by the isentropic efficiency ()η).

$$W_{\mathrm{S}} = \eta W_{\mathrm{S,isoS}} \tag{3.25}$$

Figure 3.11 shows the typical available isentropic efficiency of steam turboexpanders in respect to the rated turbine power. This cloud was constructed from compiled points collected from some available literature ([3], [4], [5] and [6]) and from authors' data.

Figure 3.11: Typical efficiency in respect to Rated Power of turbine



Source: Compiled from [3], [4], [5], [6] and author data

Equation 3.26 was fitted to data and it is used for the further sensitivity calculations.

$$\eta = 0.1105 \cdot W^{0.2319} \tag{3.26}$$

The savings are calculated as Equation 3.27.

$$\text{Savings} = C_{\text{power}} \cdot W_s - C_{\text{maint}} \tag{3.27}$$

where maintenance cost (C_{maint}) is assumed equal to 3% of total investment per year.

This work aims to calculate ranges of preliminary economic feasibility of a steam turboexpander.

References

[1] WAGNER, W. *et al.* **The IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam.** ASME J. Eng. Gas Turbines and Power. v. 122, pp. 150-182, 2000.

[2] SPANG, B. **water97 v13: A collection of Visual Basic functions for calculating properties of water and steam.** Version 1.3. Software, 2002.

[3] POPE, J. E. **Rules of Thumb for Mechanical Engineers**. Gulf Professional Publishing, 1996. 406 p.

[4] BRANAN, C. **Rules of Thumb for Chemical Engineers**. 4th ed. Gulf Professional Publishing, 2005.

[5] FORSTHOFFER, W. **Forsthoffer's Best Practice Handbook for Rotating Machinery**. Butterworth-Heinemann, 2011. 672 p.

[6] PERRY, R. H.; GREEN, D. W.; MALONEY, J. O. (orgs.). **Perry's Chemical Engineers' Handbook**. 7th ed. New York: McGraw-Hill, 2008.

List of symbols

Symbol	Description	Unit
$\dot{m}$	Valve mass flow	kg/h
$\dot{m}_{\mathrm{T}}$	Turbine mass flow	kg/h
P_1	Inlet pressure (absolute)	bar a
T_1	Inlet temperature	°C
T_2	Outlet temperature from real expansion	°C
h_1	Steam specific enthalpy at inlet state	kJ/kg
s_1	Steam specific entropy at inlet state	kJ/kg/°C
P_2	Outlet pressure (absolute)	bar a
$T_{2,isoH}$	Outlet temperature from isoenthalpy expansion	°C
$T_{2,isoS}$	Outlet temperature from isentropic expansion	°C
h_2	Steam specific enthalpy at outlet state	kJ/kg
$h_{2,S}$	Steam specific enthalpy at outlet state (isentropic)	kJ/kg
L	Pipeline length	m
$W_{S,isoS}$	Produced work from isentropic expansion	kW
W_S	Produced work from real expansion	kW
$x_{2,isoS}$	Outlet steam quality from isentropic expansion	-
x_2	Outlet steam quality from real expansion	-
η_{est}	Estimated isentropic efficiency of turbine	-
η	Chosen isentropic efficiency of turbine	-
CEPCI	Chemical Engineering Plant Cost Index	-

3.5.3 Steam thermocompression

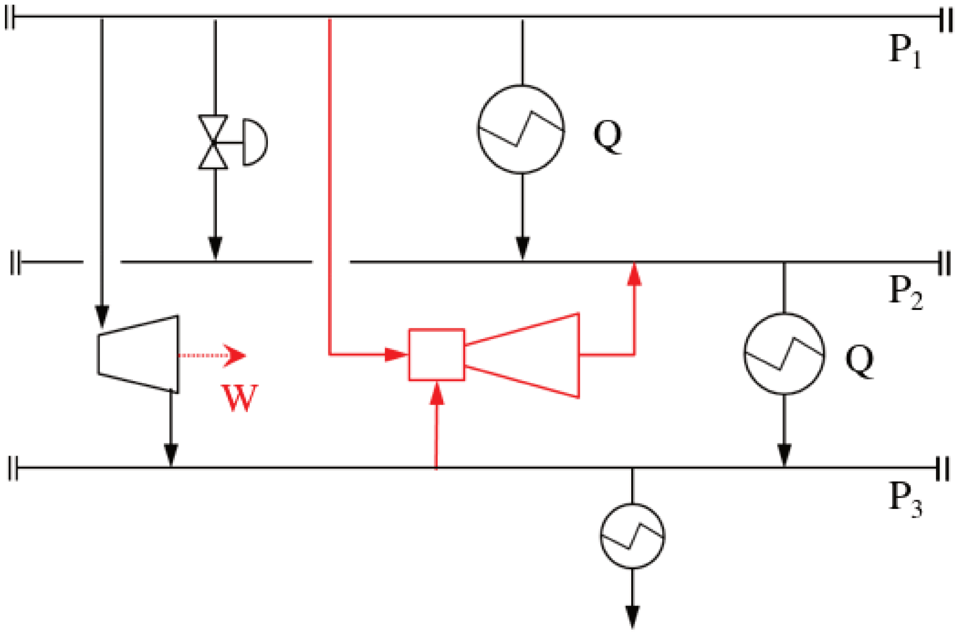
The steam thermocompression consists in using a steam jet ejector for recovery of low pressure steam (suction) by using high pressure steam (motive), obtaining medium pressure steam (discharge). It is an operation of interest to energy savings in processes.

In this work, models which correlate ratio of driving steam flow by suction steam flow with the ratios of compression and expansion in steam ejectors and their cost curves were analyzed. The models were validated with data available from manufacturers' catalogs and one was selected for the study as it was more appropriate to represent the actual data and a wider range of conditions.

This tool provides a quick preliminary estimation for technico-economic feasibility of a new thermocompressor installation.

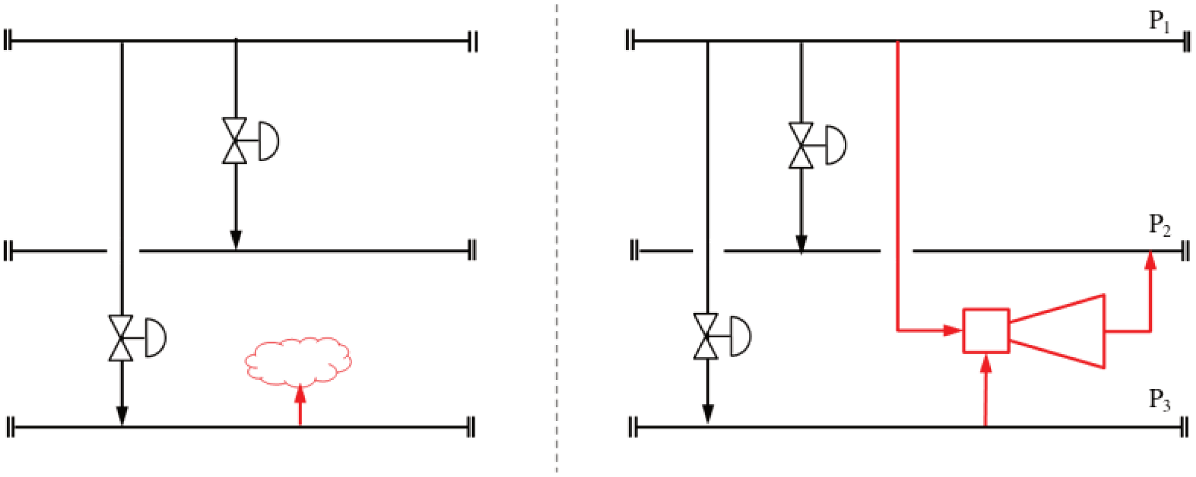
Figure 3.12 shows a generic and simplified steam network comprised of heat loads, steam turbine and the thermocompressor.

Figure 3.12: Steam jet ejector installation setup



There are two main situations where installing a thermocompressor can be advantageous. The first, as shown on Figure 3.13, happens when there is an excess of low pressure steam available, and it needs to be relieved to atmosphere or condensed.

Figure 3.13: Steam jet ejector installation setup



The second, as shown on Figure 3.14, evolves a turbine with idle capacity due to an excess of low pressure vapor. As a consequence, this equipment is not able to reduce a higher steam flow. In this situation, some of this low pressure steam can be re-compressed to a level where exists consumption, allowing a better energy use for the steam turbine.

Figure 3.14: Steam jet ejector installation setup

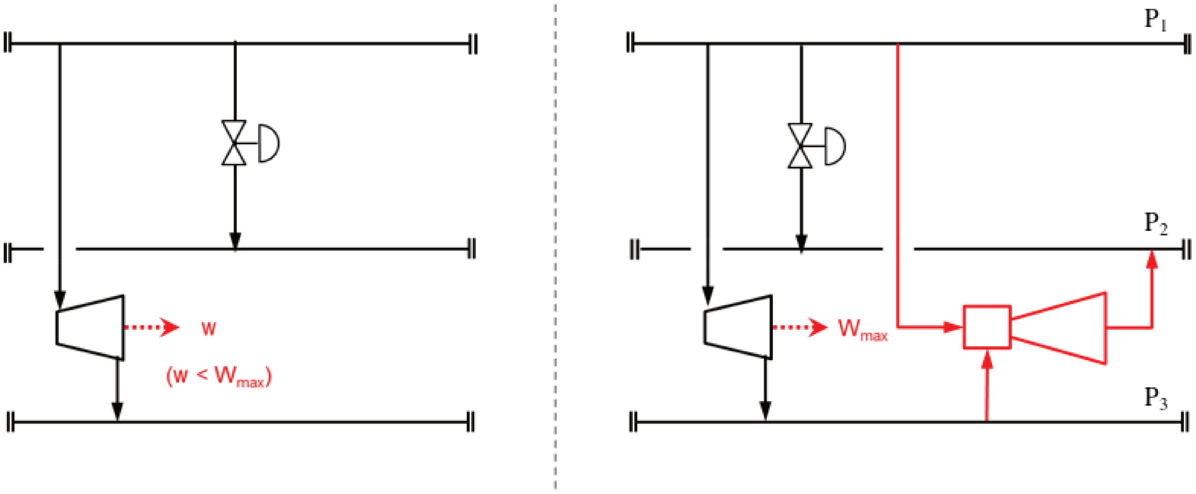
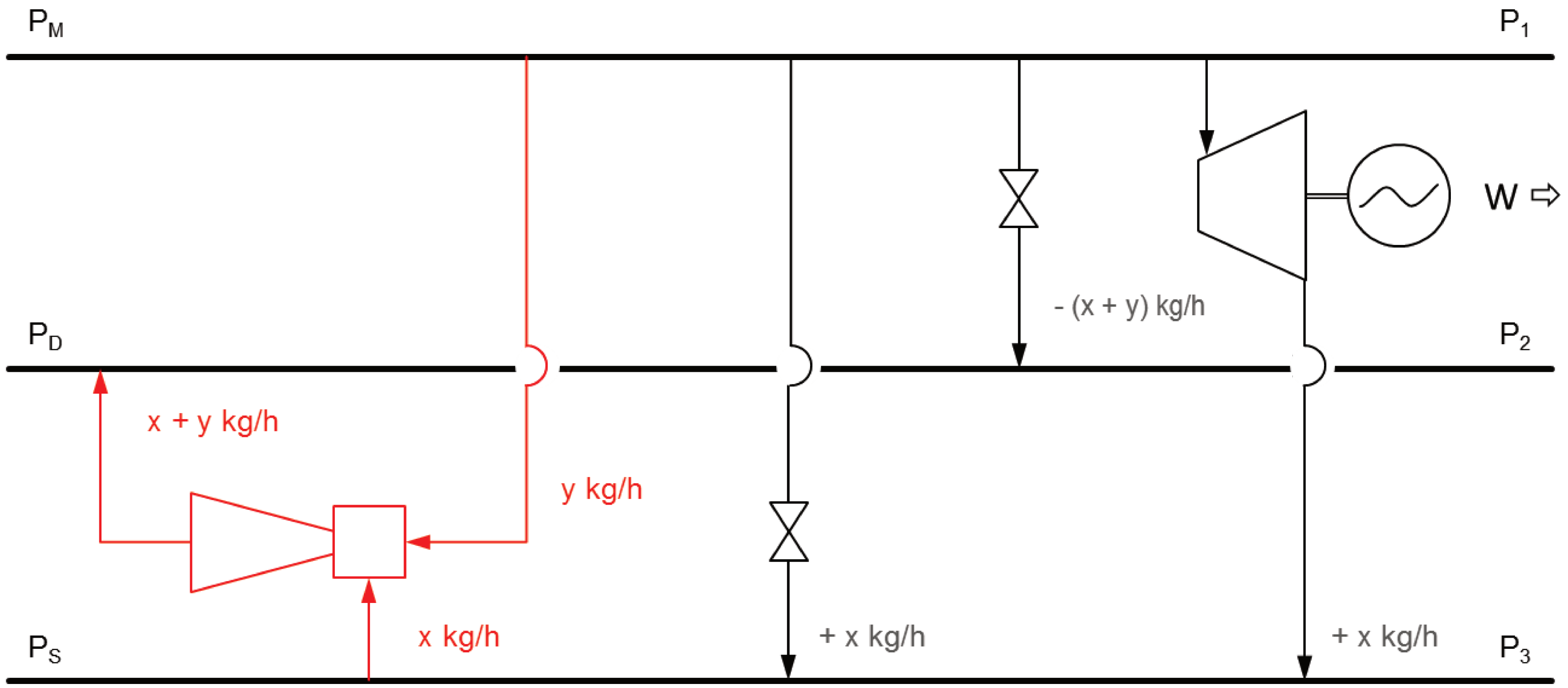


Figure 3.15 represents a simplified steam network with 3 pressure levels and a generic topology including a steam turbine, reduction valves and a thermocompressor. The demand balance is described in the drawing, showing the impact of the installation of a thermocompressor for low pressure steam upgrading.

Figure 3.15: Simplified steam network with 3 pressure levels



Assumptions

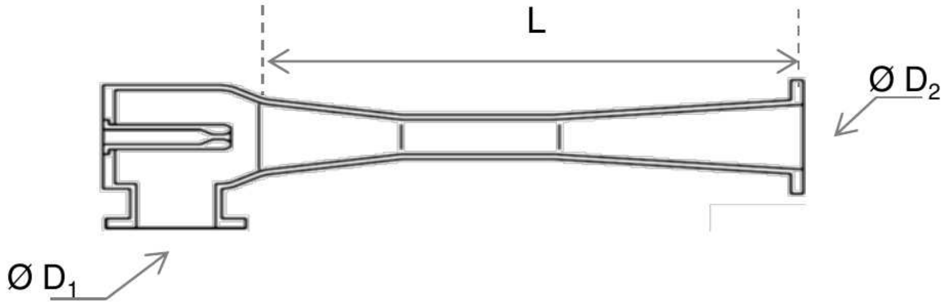
In order to keep the cost and performance models as simple as possible, some simplifying assumptions were taken, as follow:

- Motive steam is superheated
- The purchase cost of the ejector is function of inlet nozzle diameter and its length, as shown in Equation 3.28 and Figure 3.16.

$$C_{\text{ejector}} = f(D_2, L) \tag{3.28}$$

In order to make an approach sizing of the equipment, the relation of Power (1994) was used.

Figure 3.16: Key dimensions of a steam jet ejector

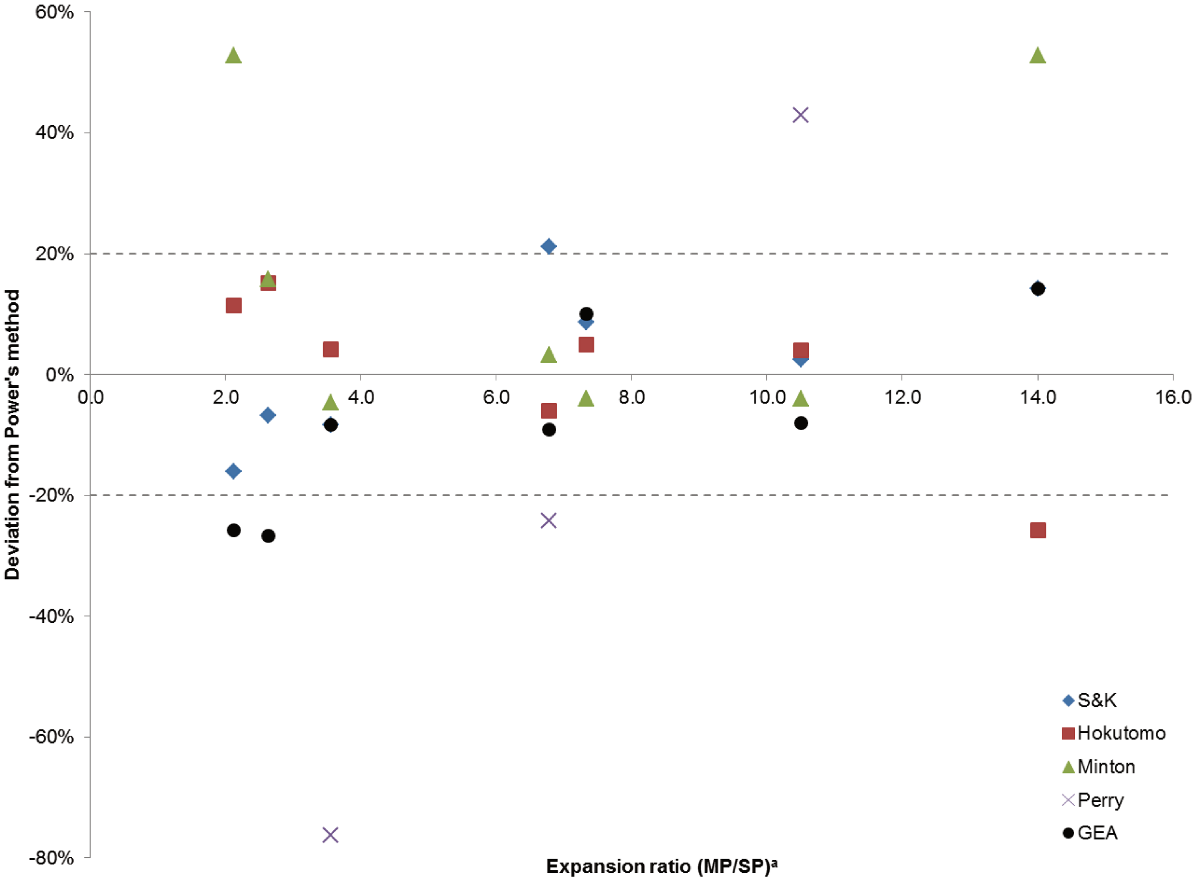


Model assessment and validation

In this work, the graphical method from Power (1994) (see Figure 2.3) was implemented computationally in order to automate the process of reading and selection of the curves. The model was checked against data available from manufacturers' catalogs and one was selected for the study as it was more appropriate to represent the actual data and a wider range of conditions.

The tool developed using Power’s model has been tested against some sources[2] commonly used to estimate thermocompression performance.

Figure 3.17: Deviation of Expansion Ratio (ER) from Power’s model for some sources



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[2] References:

[1] S&K. **Schutte & Koerting - Performance Data on Jet Compressors**.

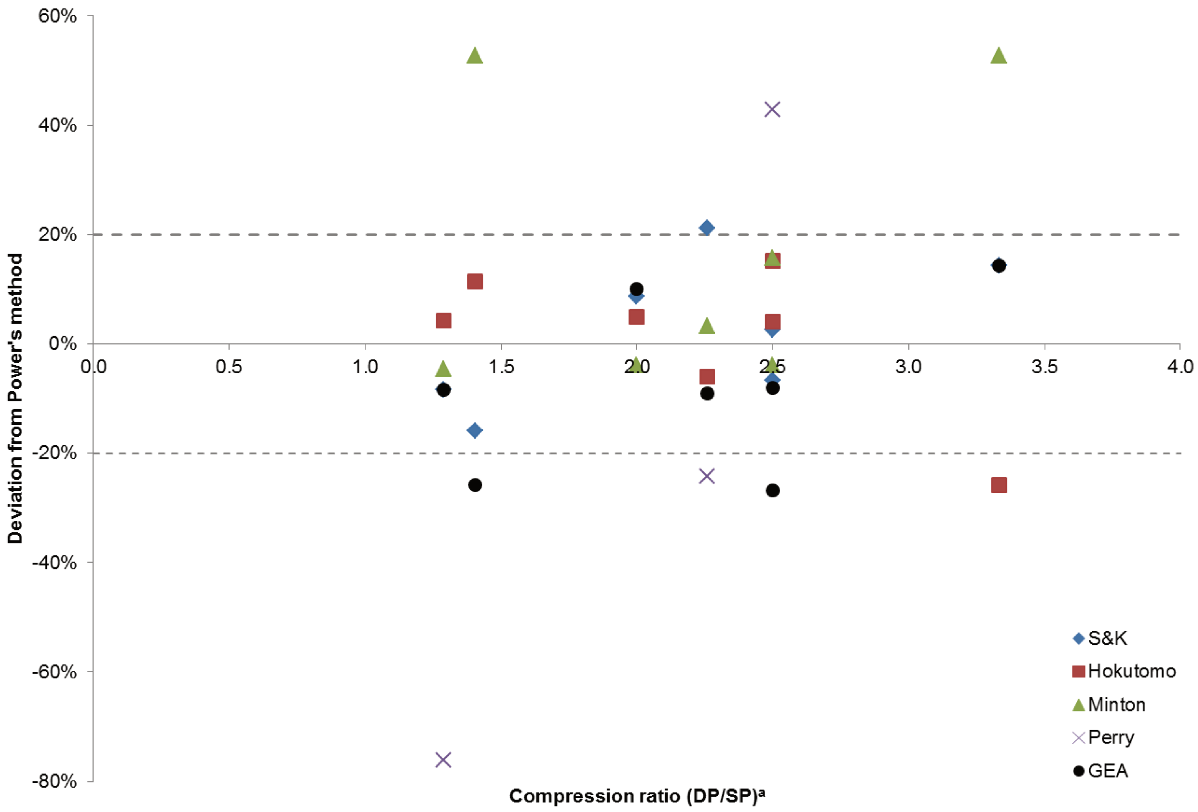
[2] HOKUTOMO. **Star Jet Thermocompressors JC catalog curves**.

[3] MINTON, P. E. **Handbook of Evaporation Technology.** Noyes Publications, 1986.

[4] PERRY, R. H.; GREEN, D. W.; MALONEY, J. O. (orgs.). **Perry’s Chemical Engineers’ Handbook.** 7th ed. New York: McGraw-Hill, 2008.

[5] GEA**. Evaporation Technology using Mechanical Vapour Recompression.**

Figure 3.18: Deviation of Compression Ratio (CR) from Power's model for some sources



More than 75% of the compared points (22 out of 30) were within a ±20% deviation range from the predicted performance, this was considered reasonably acceptable for early stage assessments.

Apparently, the error dispersion is uniform along all range of the values of ER and CR evaluated, indicating that the model is equally robust over all validity range.

List of symbols

Symbol	Description	Unit
MP	Motive (high pressure) steam pressure	barg
SP	Suction (low pressure) steam pressure	barg
DP	Discharge (medium pressure) steam pressure	barg
CR	Compression ratio (DP / SP)	-
ER	Expansion ratio (MP / SP)	-
MW	Motive steam mass flow rate	kg/h
SW	Suction steam mass flow rate	kg/h
DW	Discharge steam mass flow rate	kg/h
L	Overall length	mm
D_1	Suction nozzle diameter	in
D_2	Discharge nozzle diameter	in
C_{ejector}	Purchased cost of ejector	k$

3.6 Utilities systems

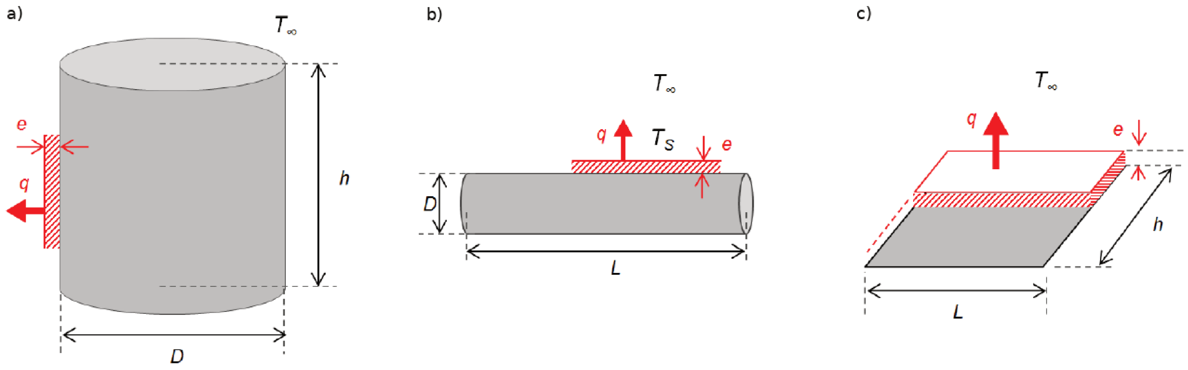
3.6.1 Thermal insulation

Typical situations have been simulated in order to analyze the sensitivity of optimal insulation thickness and give general directives to guide the engineer during early stages design.

For sake of simplicity, the heat loss phenomena models have been applied to representative surfaces: horizontal cylindrical surfaces, vertical cylindrical surfaces and horizontal flat surfaces, as shown on Figure 3.19.

Figure 3.19: Simple schematic of the models of heat loss

a) Vertical cylinder, b) Horizontal cylinder and c) Flat plate



Assumptions

From the heat transfer models used, it's intended that:

- The horizontal cylindrical model represent, with reasonable accuracy, the behavior of long horizontal pipes;
- The vertical cylindrical model can represent, with fair accuracy, large vertical tanks, however, the convection model used here can give inaccurate results for small diameter tanks or vertical pipes;
- The flat plate model can represent other equipment surfaces.

Model

1. Convection

Thermal convection model:

$$Q_C = hA\left(T_s - T_\infty\right) \tag{3.29}$$

Convective heat transfer coefficient estimation

$$h = \frac{Nu \cdot k}{L} \tag{3.30}$$

Nusselt number estimation (natural convection)

- Horizontal cylinder

$$Nu = \left\{0.60 + \frac{0.387 Ra_D^{1/6}}{\left[1 + \left(\frac{0.559}{Pr}\right)^{9/16}\right]^{8/27}}\right\}^2 \tag{3.31}$$

- Vertical surfaces (small curvature)

$$Nu = \left\{0.825 + \frac{0.387 Ra_L^{1/6}}{\left[1 + \left(\frac{0.492}{Pr}\right)^{9/16}\right]^{8/27}}\right\}^2 \tag{3.32}$$

where Ra is the Rayleigh number, given by:

$$Ra = \frac{g\left(\frac{2}{T_\infty + T}\right)\left(T_s - T_\infty\right) L^3}{\alpha \nu} \tag{3.33}$$

Nusselt number estimation (forced convection)

- Cylinder (Hilpert's correlation):

$$Nu = C Re^m Pr^{0.37} \tag{3.34}$$

where C and m are function of Reynolds number and are tabulated below:

Re	C	m
0.4-4	0.989	0.330
4-40	0.911	0.385
40-4000	0.683	0.466
4000-40,000	0.193	0.618
40,000-400,000	0.027	0.805

Source: INCROPERA and DEWITT (2011)

- Vertical surfaces (small curvature)

$$Nu = \begin{cases} 0.664Re^{0.5}Pr^{0.33},\ Re < 5 \times 10^5 \\ (0.037Re^{0.8} - 871)Pr^{0.33},\ 5 \times 10^5 < Re < 1 \times 10^8 \end{cases} \tag{3.35}$$

2. Radiation (black body radiation)

Stefan-Boltzmann model:

$$Q_R = \sigma \varepsilon A \left(T_s^4 - T_\infty^4\right) \tag{3.36}$$

3. Surface temperature with insulation

Plane surfaces

$$T_{s,i} = \frac{hT_\infty + T_S \dfrac{k_i}{e}}{h + \dfrac{k_i}{e}} \tag{3.37}$$

Cylindrical surfaces

$$T_{s,i} = \frac{k_i T + h\left(\frac{D}{2} + e\right) \ln\left(\dfrac{\frac{D}{2} + e}{\frac{D}{2}}\right) T_\infty}{h\left(\frac{D}{2} + e\right) \ln\left(\dfrac{\frac{D}{2} + e}{\frac{D}{2}}\right) + k_i} \tag{3.38}$$

4. Wet insulation

Fibrous insulation material

$$k_{i,\text{eff}} = f_w \cdot 24 \cdot (1 + k_i) \tag{3.39}$$

Non-fibrous insulation material

$$k_{i,\text{eff}} = f_w \cdot 14 \cdot (1 + k_i) \tag{3.40}$$

References

[1] INCROPERA, F. P.; DEWITT, D. P. **Fundamentals of heat and mass transfer**, 7th ed, Wiley & Sons, 2011. 1080p.

List of symbols

Symbol	Description	Unit
T_∞	Ambient temperature	°C
T_S	Bare surface temperature	°C
T_{Si}	Temperature at insulation wall	°C
T_f	Film temperature	°C
e	Insulation thickness	mm
I_{sun}	Mean solar irradiance	$\mathrm{W/m^2}$
DLH	Daylight hours	h/day
v_∞	Mean air speed	km/h
OT	Operating time	h/year
Re	Reynolds number	-
Ra	Rayleigh number	-
Nu	Nusselt number	-
Pr	Prandtl number	-
Q_C	Heat loss due convection	W
Q_R	Heat loss due radiation	W
Q_T	Total heat loss	W
Q_i	Total heat loss (insulated)	W
α	Fluid thermal diffusivity	$\mathrm{m^2/s}$
ν	Kinematic viscosity	$\mathrm{m^2/s}$
k_i	Insulation thermal conductivity	W/(m K)
$k_{i,\text{eff}}$	Effective wet insulation thermal conductivity	W/(m K)
h	Convective heat transfer coefficient	$\mathrm{W/(m^2\ K)}$
ε	Emissivity	-
σ	Stefan-Boltzmann constant	$\mathrm{W/(m^2\ K^4)}$
f_w	Moisture volume fraction	-

Chapter 4

Results and Discussion

4.1 General results

Various systems and unit operations which compose an industrial chemical process, including chemical transformation processes (reaction), separation, heat exchange, fluid transport and allocation of utilities were studied in order to develop simplified models and software tools for quick sizing and economic evaluation of equipment and systems.

In this chapter, the results obtained are presented accompanied by discussions about insights which can be drawn from these results, aiming to assist the process engineer on the decision to continue or not a given study on energy efficiency in early stage of design.

As in the previous chapters, each studied system is presented in sections following the layers of the onion model.

4.2 Reaction

4.2.1 Specific energy consumption in chemical processes

Physical reasoning for the correlation

Considering a thermally ideal process in which all released energy could be reused in the process, without losses:

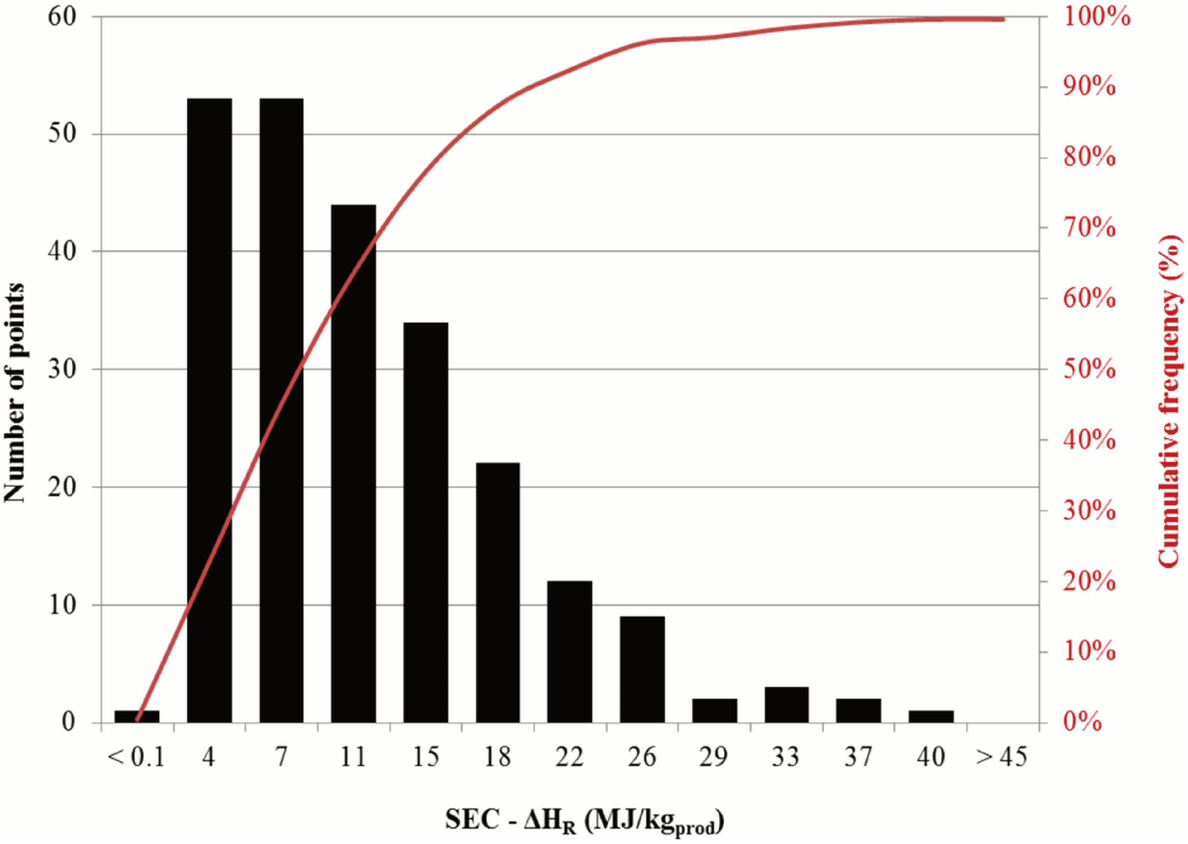
- In the case of ideal exothermic processes, it is expected that all the energy released due to reaction would be recovered without losses and it would be possible to export all the surplus energy;
- In the case of ideal endothermic reactions, on the other hand, only the energy needed to drive and sustain the reaction would be required.

Therefore ideal processes would lie on the line $SEC = \Delta H^\circ_\mathrm{R}$. The vertical distances between the plotted points and the line $SEC = \Delta H^\circ_\mathrm{R}$ suggest deviation from thermal ideality of the corresponding processes. This additional consumption is probably due to non-reaction steps such as operations of momentum transfer, heating, synthesis selectivity, separations, exothermic reactions running at low temperatures, losses to the environment, among other factors.

The assumption that thermal energy released during the reaction can be recovered, by energy integration or generation of work, depends strongly on the temperature level at which the reactions take place. For example, the production of Maleic Anhydride from the oxidation of Butane or Benzene runs near to $400\,^\circ\mathrm{C}$, releasing large amounts of high quality energy that could be exported and used on other process operations. On the other hand, bio-processes and other mild temperature reaction processes can also release huge amounts of energy, but at temperatures near to the environment, increasing the difficulty of heat recovery.

In Figure 4.1 we show the distribution of collected data regarding the additional energy consumption ($SEC - \Delta H^\circ_\mathrm{R}$). It can be seen from the histogram and from the cumulative frequency shown that more than 90% of the processes studied present values of additional energy consumption lower than 20 MJ/kg product.

Figure 4.1: Distribution of bands of additional energy consumption ($SEC - \Delta H_{\mathrm{R}}^{\circ}$)

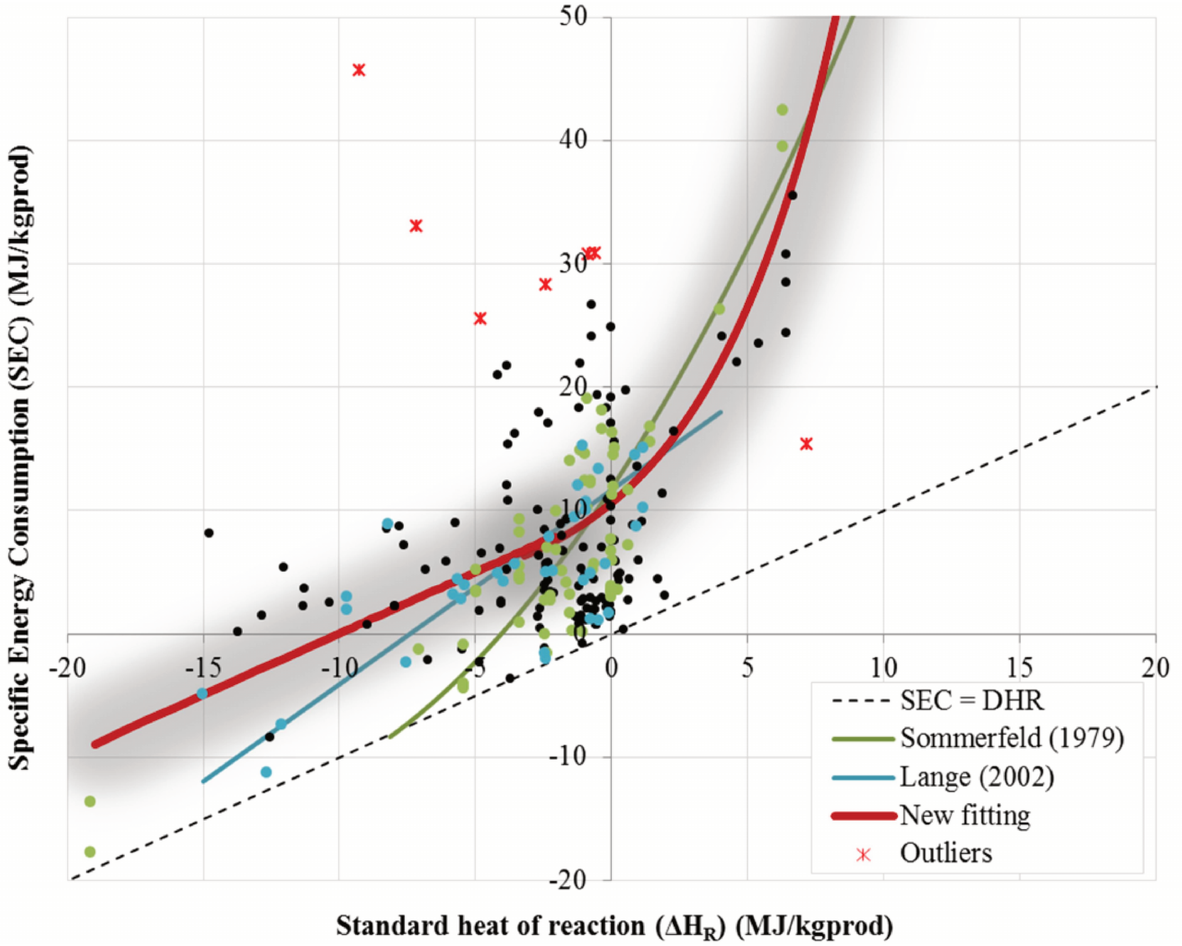


Despite not being an exhaustive collection of points, it is possible to notice from Figure 3.4 that the $\Delta H_{\mathrm{R}}^{\circ}$ of typical chemical, petrochemical and specialties reactions fit in the range between -20 MJ/kg product for the most exothermic reactions to 8 MJ/kg product for the most endothermic ones, the exothermic reactions being the great majority. This work proposes a new correlation between the SEC and the $\Delta H_{\mathrm{R}}^{\circ}$ as shown in Equation 4.1.

$$SEC = \begin{cases} 1700 + 9000 \exp\left(2.05 \cdot 10^{-4} \Delta H_{\mathrm{R}}^{\circ}\right) & \text{if } \Delta H_{\mathrm{R}}^{\circ} \geq -2.5\,\mathrm{MJ/kg} \\ 10000 + \Delta H_{\mathrm{R}}^{\circ} & \text{if } \Delta H_{\mathrm{R}}^{\circ} < -2.5\,\mathrm{MJ/kg} \end{cases} \tag{4.1}$$

The reported SEC values, the predicted SEC with Equation 4.1 and their respective deviations are listed in Table A.1. 97.5% (232 out of 238 points) of deviations between estimated (SEC') and reported SEC were below two standard deviations (σ) from the reported SEC data (9000 MJ/kg of product). The points which were above two standards deviations are marked as crosses (×) in Figure 4.2. It is out of the scope of this work to reason about the causes of the drifted points.

Figure 4.2: Specific Energy Consumption versus Standard Enthalpy of reaction: new fitting proposed for all data-sets



Considering the additional data gathered in this work, the observation of Sommerfeld and White (1979) that “this deviation is greater than one would like” and that “it is certainly reasonable in view of the inherent scattering of the raw data” still remains valid.

Validation and restrictions

The data presented in Figure 3.4 shows that values for both are located in the same cloud of points when compared to the total specific consumption of chemical processes. Therefore the equation can be considered valid for both $\Delta H^\circ_\mathrm{R}$ and $\Delta G^\circ_\mathrm{R}$. It is not the purpose of this work to construct a physical association or model between the thermodynamic characteristics of the reaction and the total specific consumption, but rather to present a statistical correlation between these data.

Special care must be taken for pathways comprising of more than one synthesis step with significant differences in enthalpy of reaction or reaction temperatures, because each of these steps would contribute positively or negatively to the overall estimate from the enthalpy difference between the products and the main raw materials.

The new correlation can be used for $\Delta H^\circ_\mathrm{R}$ and $\Delta G^\circ_\mathrm{R}$ in the range between -20 MJ/kg of product and 8 MJ/kg of product.

Conclusion

The pioneer and insightful work of Sommerfeld and White (1979) has been revisited to enhance its usefulness and to verify its validity with a wider set of data.

A new correlation between the SEC and $\Delta H^\circ_\mathrm{R}$ of a product or process has been proposed aiming to provide a quick first estimate of the SEC at early stages of process development and design from basic reaction synthesis data. 172 additional data were gathered for several types of chemical industry products, such as basic chemicals, petrochemicals, solvents and specialties, coming from reactive processes or not, and analyzed along with the original work of Sommerfeld and White (1979) with 66 data points. This correlation is useful for the early estimation of manufacturing costs of new processes using early synthesis information easily found on literature and from fundamentals.

In a wide range, this work corroborated the result found by Sommerfeld and White (1979). The new correlation was fitted to a complementary data-sets, listed in Table A.1, including chemical specialties and some processes from newer literature, conciliating previous works.

It also can be used to predict values of SEC for highly exothermic reactions more realistically than those predicted by the quadratic function proposed by Sommerfeld and White (1979).

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4.3 Separation operations

4.3.1 Heat pump assisted distillation

Base case

The following analysis assumed the base case shown on Table 4.1.

Table 4.1: Heat pump assisted distillation - base case conditions

Parameter	Value
Top temperature (T_{top})	$90\,°\mathrm{C}$
Bottom temperature (T_{bot})	$105\,°\mathrm{C}$
Enthalpy of vaporization at top (λ_V)	$150\,\mathrm{kcal/kg}$
Vapor Cp/Cv	1.116
Vapor molecular mass	$58\,\mathrm{kg/kmol}$
Required reboiler duty	$980\,\mathrm{Mcal/h}$

The values assumed on Table 4.1 are based on an industrial distillation of a mixture of acetone and water.

When applicable, the costs of power and steam were used from Table 3.2, which are realistic figures for Brazilian market.

Sensitivity analysis

Using the tool described in section 3.3.1, some sensitivity studies were performed as follow:

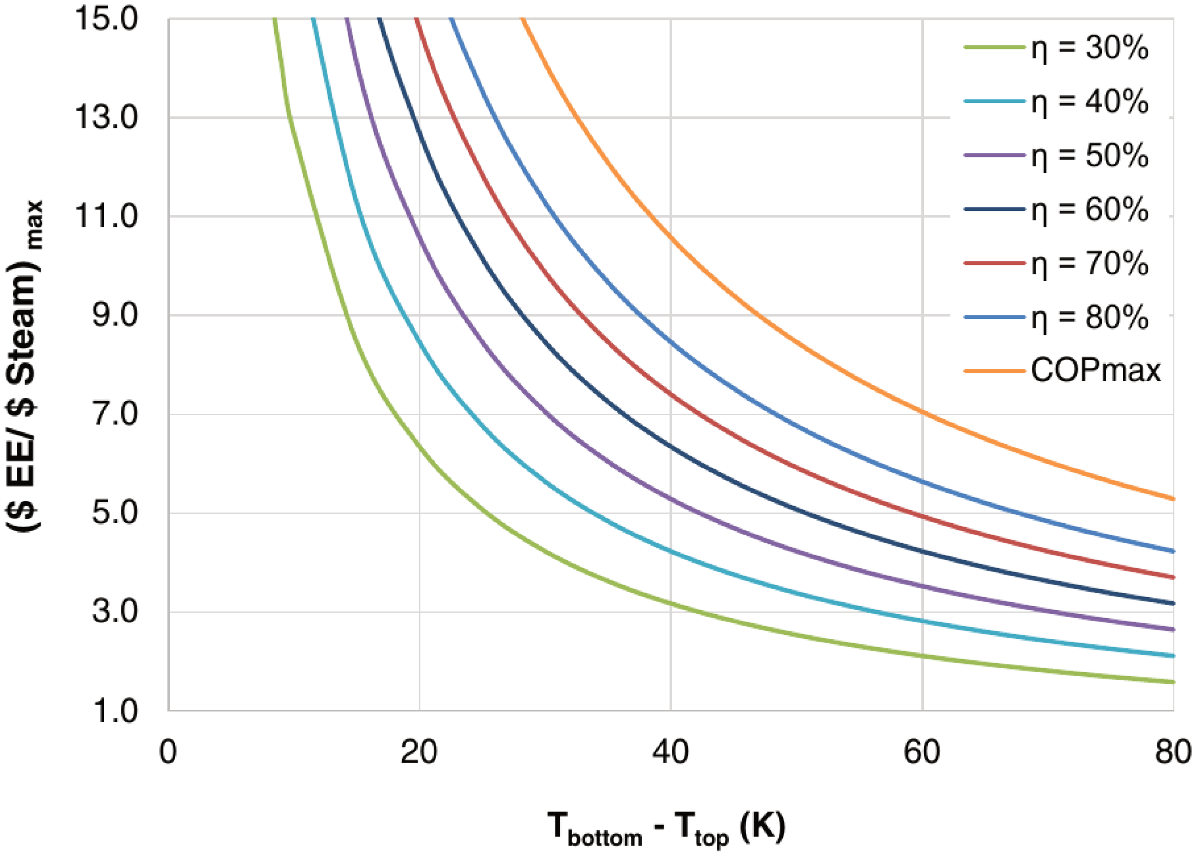
Sensitivity 1 - Break-even energy cost versus Top - Bottom temperature difference

On this first sensitivity analysis, the economical feasibility of applying heat pump assisted distillation for different separations systems were evaluated.

Figure 4.3 shows the maximum ratio between electricity cost and steam cost (both in the same energy basis) to give a positive saving (infinite simple payback) in respect to the temperature difference between bottom and top ($\Delta T_{\text{b-t}} = T_{\text{bot}} - T_{\text{top}}$).

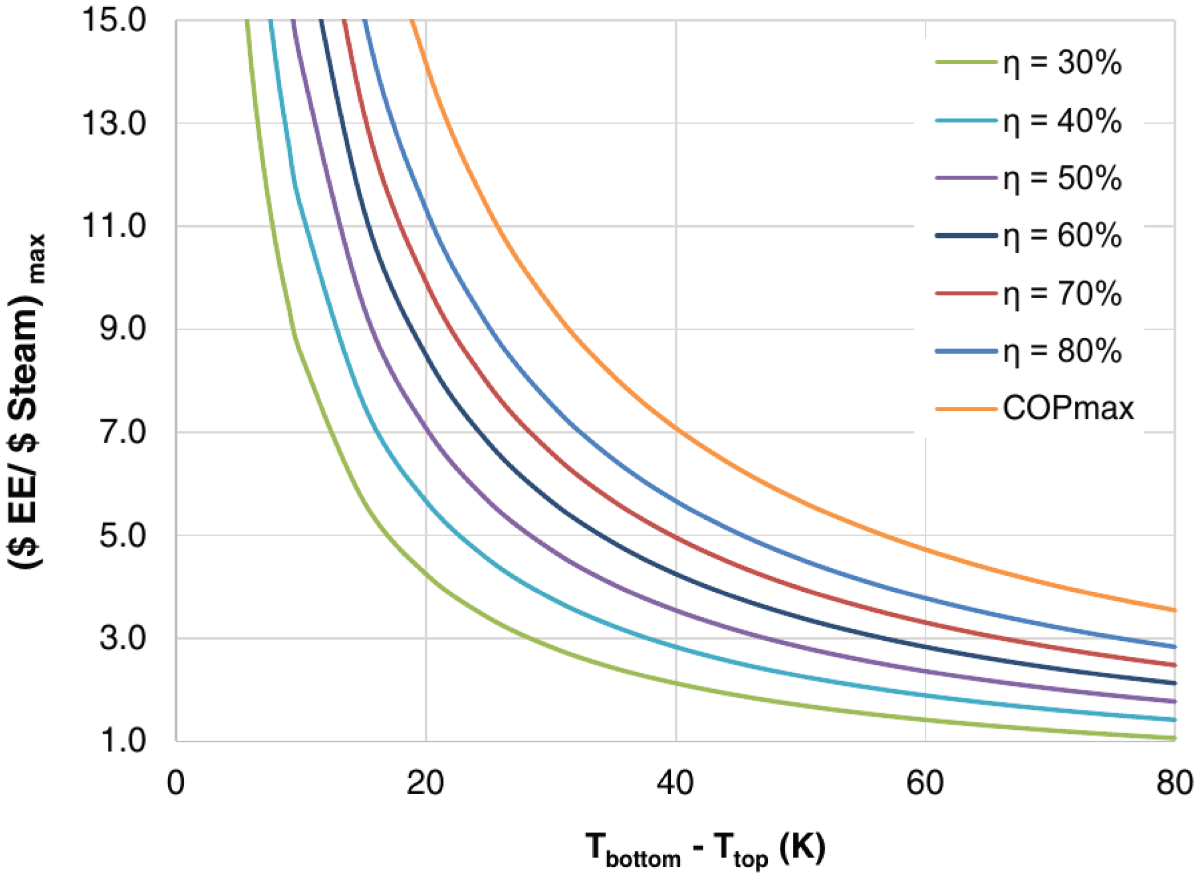
The upper outermost curve represents the system's performance at the thermodynamic maximum COP. The other lower curves express the fractions of COP_{max} with the overall system efficiency η_{over}.

Figure 4.3: Economical feasibility limit in respect to column temperature difference and energy cost ratio



Additionally, Figure 4.4 presents the curves for a economic break-even point for 3 years simple payback.

Figure 4.4: Economical feasibility for simple payback = 3 years, in respect to column temperature difference and energy cost ratio



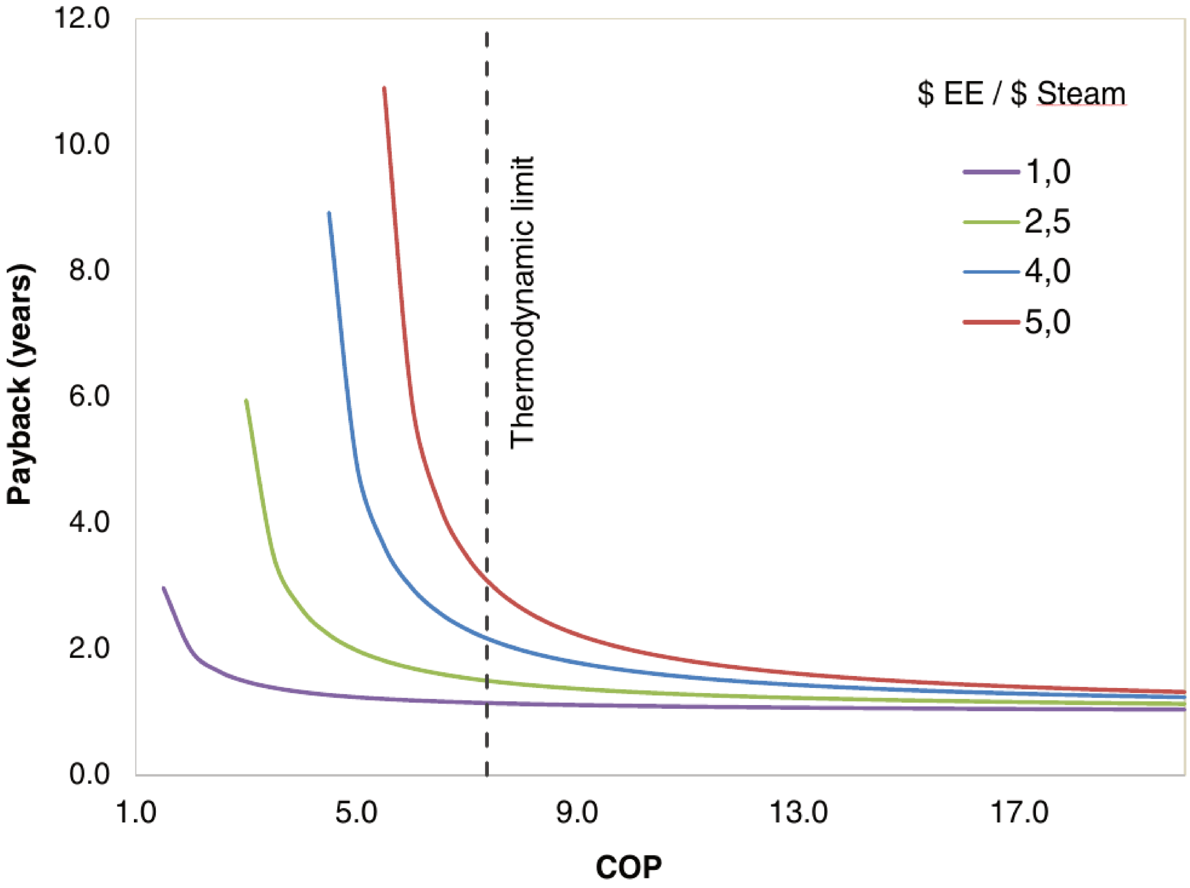
Sensitivity 2 - Payback time versus COP

The second sensitivity analysis varied COP values for different ratios between the cost of electrical energy and thermal energies ($ EE / $ Steam). The results obtained are shown on Figure 4.5.

From Figure 4.5, it can be seen that the payback time of the installation of a heat pump is strongly dependent on the relation between the cost of electric and thermal energies ($ EE / $ Steam), mainly for lower overall Coefficients of Performance (COP).

In other words, on this example, for COP values lower than, approximately, 6, the payback curves tends to be asymptotic for a given cost ratio.

Figure 4.5: Payback time in respect to heat pump's overall COP



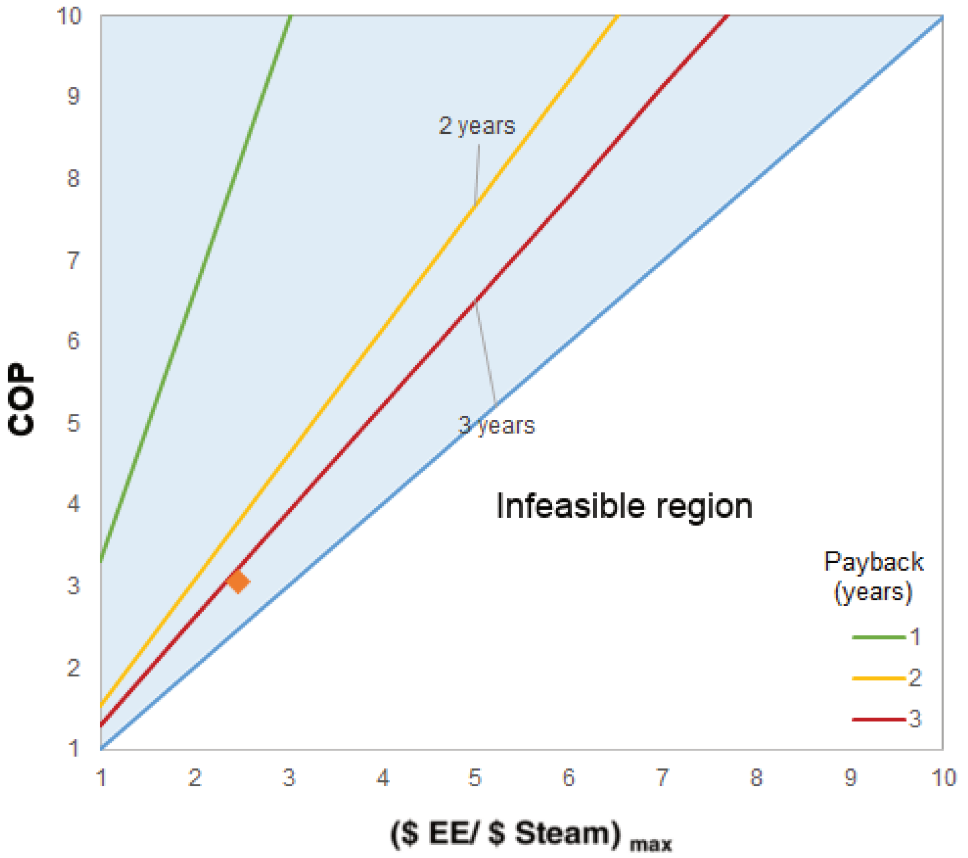
For the studied base-case, the maximum COP that the heat pump can ideally achieve is 7.2. Such efficiency is still leading to paybacks of the order of 3 years for scenarios of electricity costs above 4 times the steam cost, consequently, for this separation, heat pump assisted distillation can hardly be feasible.

As expected, the payback time is very sensitive to energy price conjuncture (ratio between prices of electrical energy and steam). In this example, the system simple payback becomes insensitive to energy price only for higher efficient systems, beyond thermodynamic limit.

These sensitivity analyses are important on assessing the potential feasibility of heat pump assisted distillation, even in the most optimistic scenarios of energy costs and attainable efficiencies.

Sensitivity 3 - Break-even COP versus energy cost ratios

Figure 4.6: Break-even COP in respect to cost ratio between electricity and steam



Conclusion

Some general conclusions can be drawn from the three sensitivity analyses carried out above.

Heat pump assisted distillation can be particularly feasible for distillation of close boiling point mixtures, since they require relatively less compression work (and consequently smaller compressors) to raise the temperature to levels that can be used in the reboiler, when compared to mixtures with higher relative volatility.

It is also worth noting that such distillations generally require larger reflux ratios and therefore higher steam consumption. What makes them attractive targets for this technology.

4.4 Heat transfer operations

4.4.1 Thermal Integration

Base case

The following analyses assumed the base-case shown on Table 4.2 and Figure 4.7.

Table 4.2: Thermal integration - base case conditions

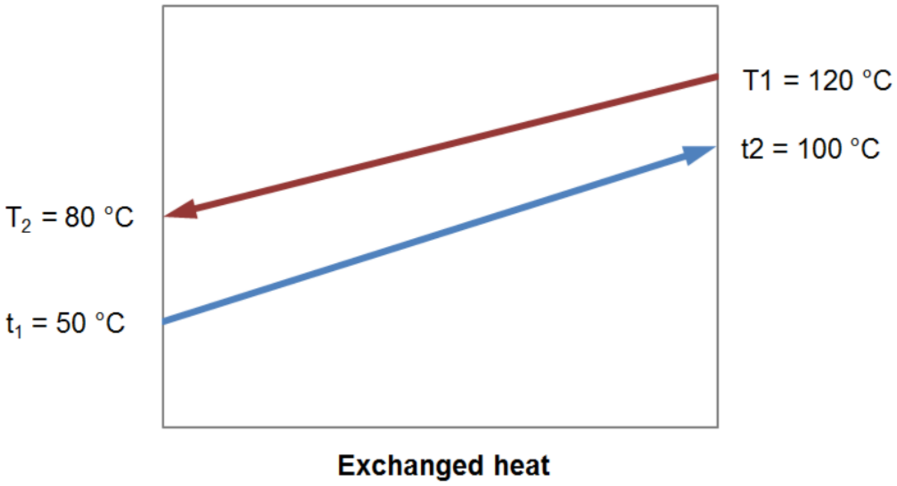
Parameter	**Value**
Flow configuration	Pure countercurrent
Cold side inlet temperature (t_1)	$50\,^\circ\mathrm{C}$
Cold side target outlet temperature (t_2)	$100\,^\circ\mathrm{C}$
Cold side mass flow ($\dot{m}_1$)	$10\,000\,\mathrm{kg/h}$
Cold side specific heat capacity ($c_{p,1}$)	$0.9\,\mathrm{kcal/kg/^\circ C}$
Hot side inlet temperature (T_1)	$120\,^\circ\mathrm{C}$
Hot side target outlet temperature (T_2)	$80\,^\circ\mathrm{C}$
Overall heat exchange coefficient (U)	$400\,\mathrm{kcal/h/m^2/^\circ C}$

These values shown on Table 4.2 were chosen arbitrarily, based on typical heating and cooling operations in industry. The overall heat exchange coefficient assumed for the integration exchanger is realistic for pumped liquid-liquid heat exchanging in shell-and-tube equipment.

The temperature range and approach temperature difference were intentionally chosen to facilitate analysis.

Figure 4.7 shows the temperature profile for both cold and hot streams along the countercurrent integration exchanger.

Figure 4.7: Integration heat exchanger profile

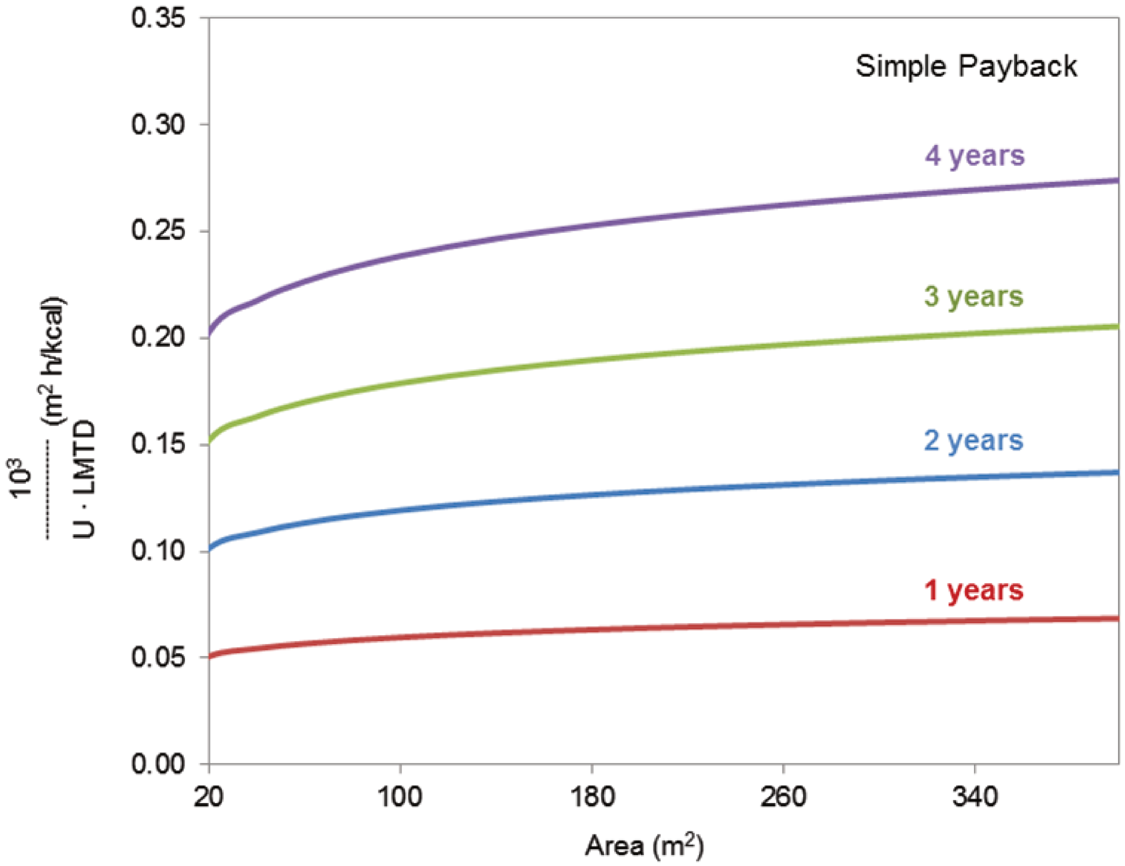


Sensitivity - Payback time versus heat exchanger parameters.

From Equation 3.20, a sensitivity analysis was performed in respect to payback time and different equipment areas, ranging from 20 to $400\,\mathrm{m}^2$.

Figure 4.8 shows four "isopayback" curves (1, 2, 3 and 4 years of simple payback).

Figure 4.8: Isopayback curves



Analysing Figure 4.8, it is possible to notice that, for a given value of vertical axis, the payback is almost irrespective to heat exchanger area. For example, increasing almost 10 times the area, for a given “y” value, the payback time barely increases half a year.

Conclusion

Payback variation is more sensitive for smaller heat exchangers (area below $30\,\mathrm{m}^2$), but the error on estimation of attractiveness seems to be reasonable in the light of cost inaccuracy of an approach estimation.

It is interesting that having only the inlet and outlet temperatures of the pair of streams and an estimation of the overall heat exchange coefficient, it is possible to estimate the attractiveness of installing a heat integration exchanger.

This result can be used to rank and select potential proposals for integrating a pair of process streams. For example, using Equation 3.19, an automated screening procedure can quickly run through several pairs and rank them.

4.5 Momentum transfer operations

4.5.1 Pumping systems

Base case

The analysis assumed the base-case shown on Table 4.3.

Table 4.3: Pumping systems - base case conditions

Parameter	**Value**
Inlet	$100\,\mathrm{m^3/h}$
Pumped fluid	water ($\rho = 1000\,\mathrm{kg/m^3}$ / $\mu = 1\,\mathrm{cP}$)
Static head	$30\,\mathrm{m}$
Pipe material	Stainless steel (SCH 10)
Pipe length	$100\,\mathrm{m}$

These values were chosen arbitrarily, based on typical pumping operations in industry.

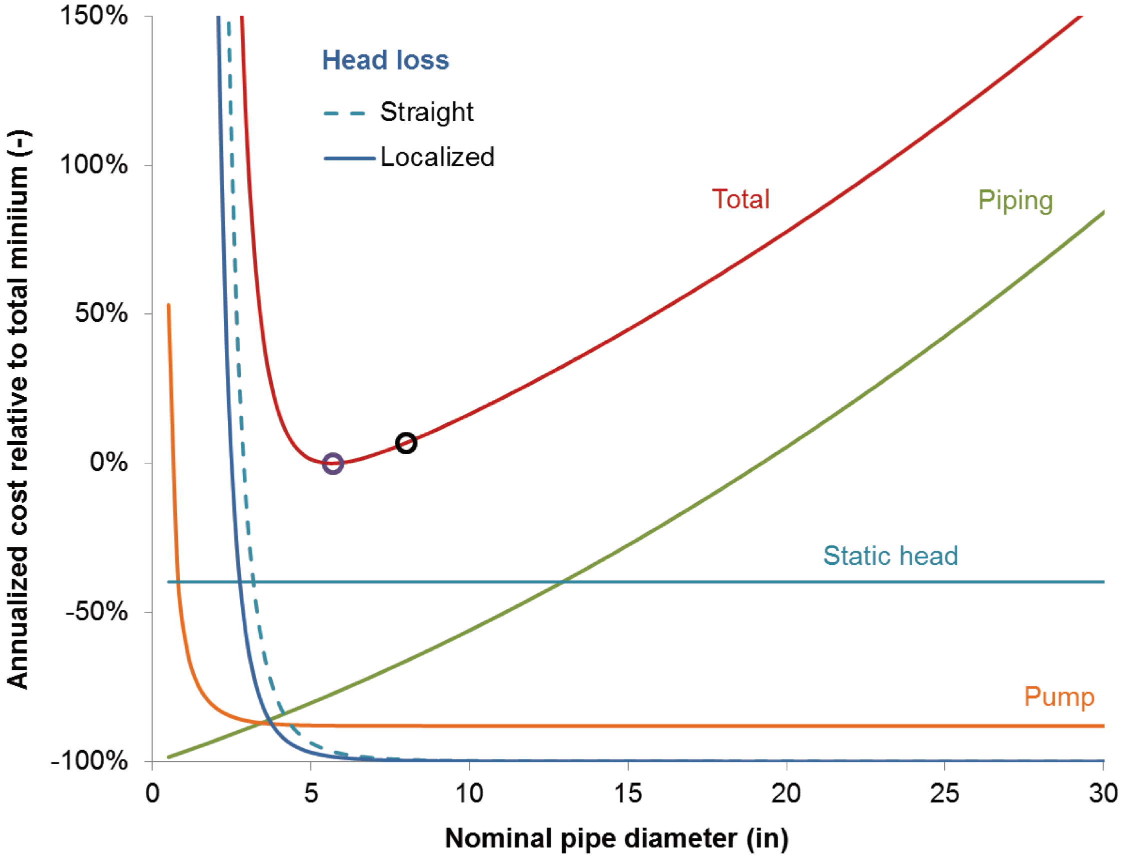
When applicable, the cost of power was used from Table 3.2, realistic figure for the Brazilian market.

Sensitivity 1 - Total annualized cost versus pipe diameter

Figure 4.9 shows a total cost curve for the system pipe + pump. The curve was splitted to their components (investment cost for pump and piping, and operating cost due to pumping energy).

The minimum energy required is represented by the "static head" curve, irrespective to pipe diameter.

Figure 4.9: Total annualized cost composition for running a pump and pipe system

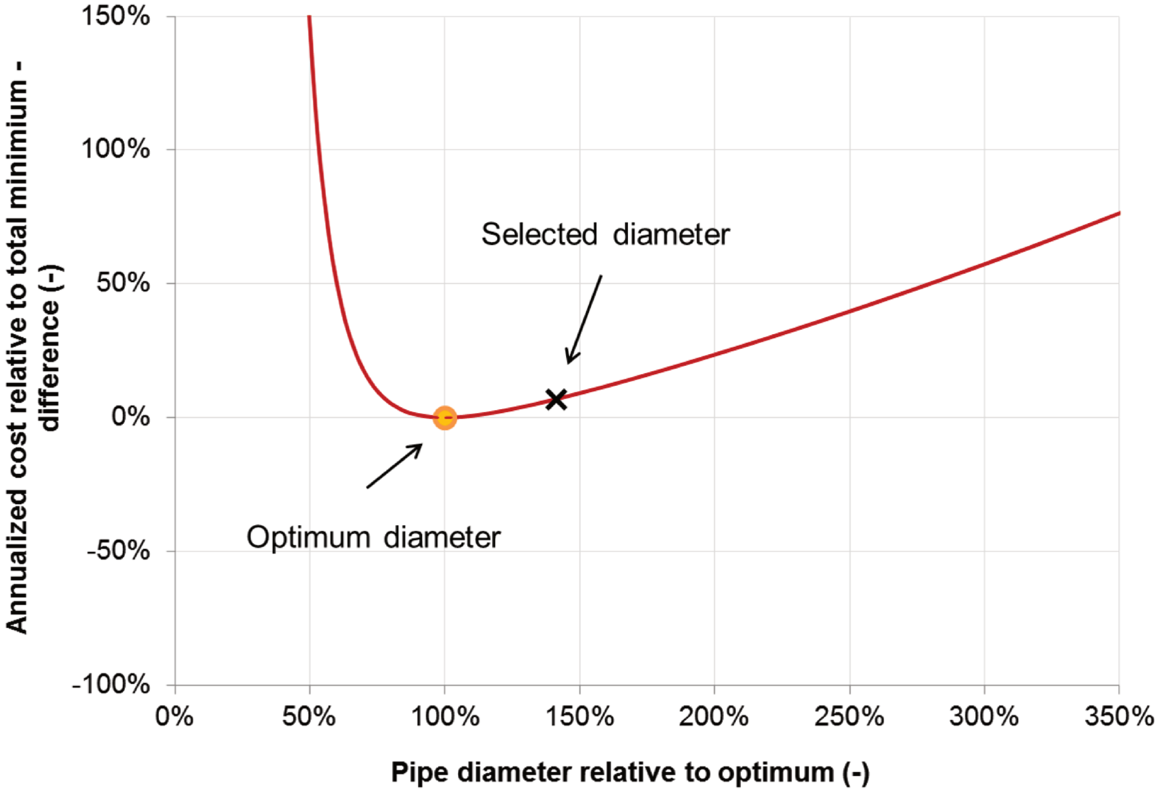


The optimum design diameter can be estimated from the total cost curve, which shows the pipe diameter that express the minimum total cost for system operation.

It is important to note that the total cost curve have an asymmetrical curvature behavior around the minimum point. The slope of the curve becomes steeper towards lower values of pipe diameter, while is more flat, towards increasing values.

This behavior gets clear on Figure 4.10 and it is due to quadratic nature of friction pressure drop in respect to diameter, against a quasi-linear function between installation cost and piping diameter.

Figure 4.10: Total annualized cost in respect to pipe diameter



Sensitivity 2 - Total annualized cost versus cost parameters

In this sensitivity analysis, the optimum diameter was calculated considering 7 scenarios of energy and material costs.

The intent here is to assess how sensitive the existing rules of thumb and heuristics for pipeline design are.

Intentionally exaggerated variations in energy and material costs (5 times the base case) were evaluated, as shown on Figure 4.11. The calculated optimal diameters and the variation in relation to the base case are shown in Table 4.4.

Figure 4.11: Total cost sensitivity in respect to energy and capital costs

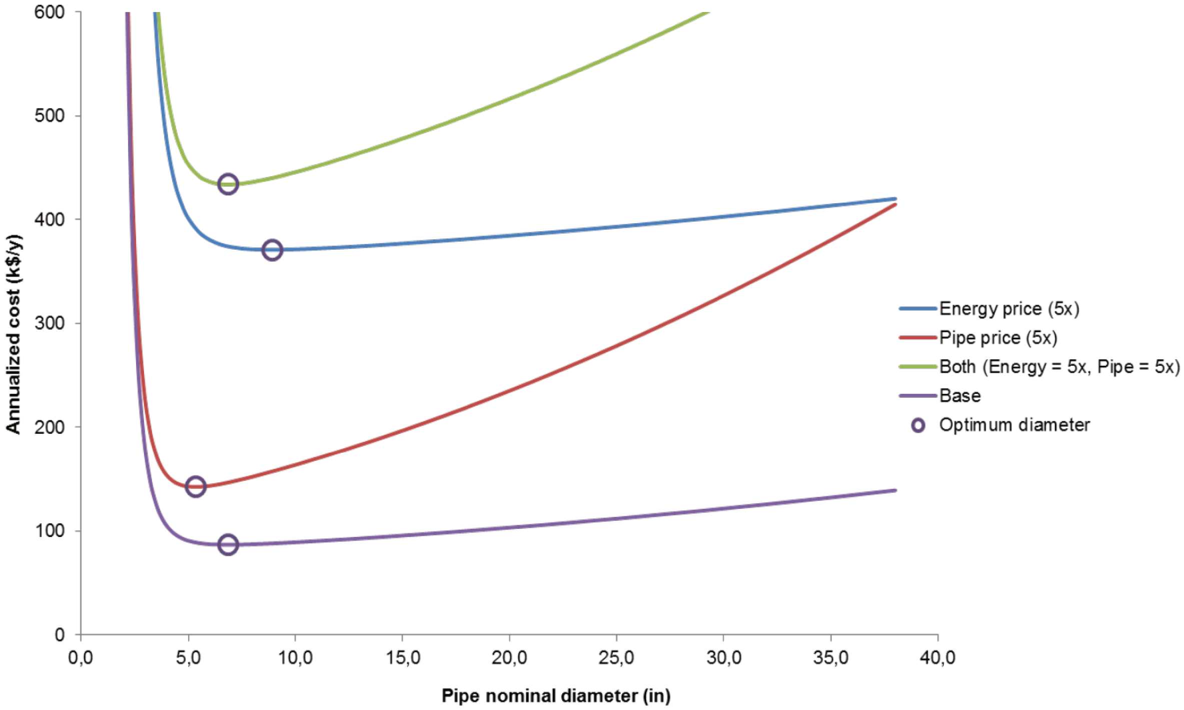


Table 4.4: Cost sensitivity of optimum pipe diameter

Case	D_{opt} (in)	ΔD (%)
Energy price (5x)	8.9	30%
Pipe price (5x)	5.3	-22%
Both (Energy = 5x, Pipe = 5x)	6.9	0%
Energy price (2x)	7.7	12%
Pipe price (2x)	6.2	-10%
Both (Energy = 2x, Pipe = 2x)	6.9	0%
Base	6.9	-

It can be seen from Figure 4.11 and Table 4.4 that the calculated optimum diameter varies little (within ± 30 %) relative to the base case.

Sensitivity 3 - Total annualized cost versus flow rate.

In this sensitivity analysis, the optimum diameters and economic velocities were calculated considering 4 different flowrates.

Figure 4.12 and Table 4.5 show how the total annualized cost is considerably sensitive to flow variations.

Figure 4.12: Total cost sensitivity in respect to flow rate

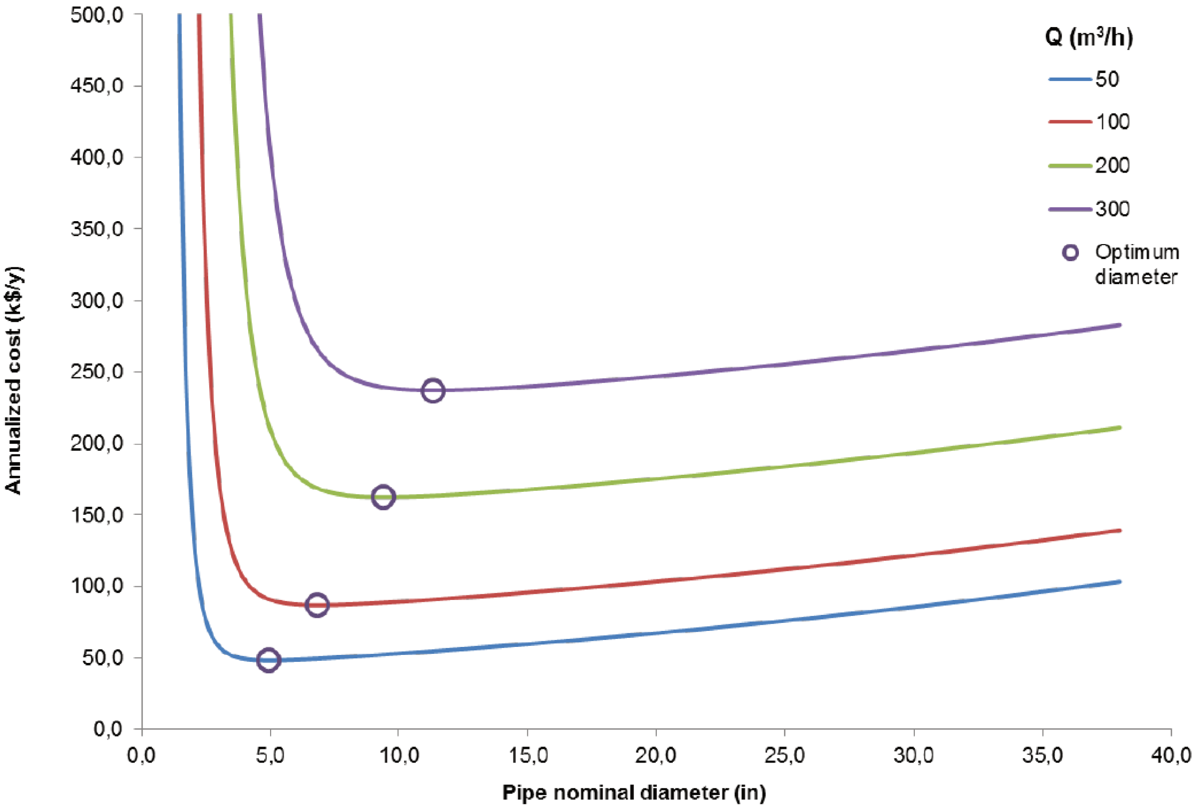


Table 4.5: Flow sensitivity of optimum pipe diameter

$Q(\mathrm{m}^3/\mathrm{h})$	$D_{\mathbf{opt}}(\mathrm{in})$	$\Delta P(\mathrm{mbar}/100\mathrm{m})$	$v_{\mathbf{opt}}(\mathrm{m/s})$
50	4.9	89	1.1
100	6.8	66	1.2
200	9.4	50	1.2
300	11.3	42	1.3

Analysing the Figure 4.12, it is possible to verify the optimum velocities doesn't change significantly (variation of less than 0.1 m/s), indicating that this rule of thumb, currently practiced in industry, can be used accurately during shortcut design.

Conclusion

System cost curve is very steep towards smaller diameters, so it is good practice to size the piping to greater than optimum diameter to accommodate future flow increases.

It is possible to verify that the optimum diameter is little sensitive with respect to energy and material prices fluctuations. Another interesting conclusion is the little sensitiveness of usual economic velocity to the flowrate. This indicates that currently used rules of thumb is still valid even for important changes on costs and are robust to a large range of flowrates.

4.5.2 Steam turboexpansion

Base case

The following analyses assumed the base case shown on Table 4.6.

Table 4.6: Steam turboexpansion - base case conditions

Parameter	**Value**
Inlet pressure (P_1)	$30\,\mathrm{barg}$
Inlet temperature (T_1)	$400\,^{\circ}\mathrm{C}$
Outlet pressure (P_2)	$9\,\mathrm{barg}$
Inlet flow rate ($\dot{m}_{\mathrm{T}}$)	$10\,\mathrm{t/h}$

These values were chosen arbitrarily, based on typical medium pressure steam expansion in industrial steam networks.

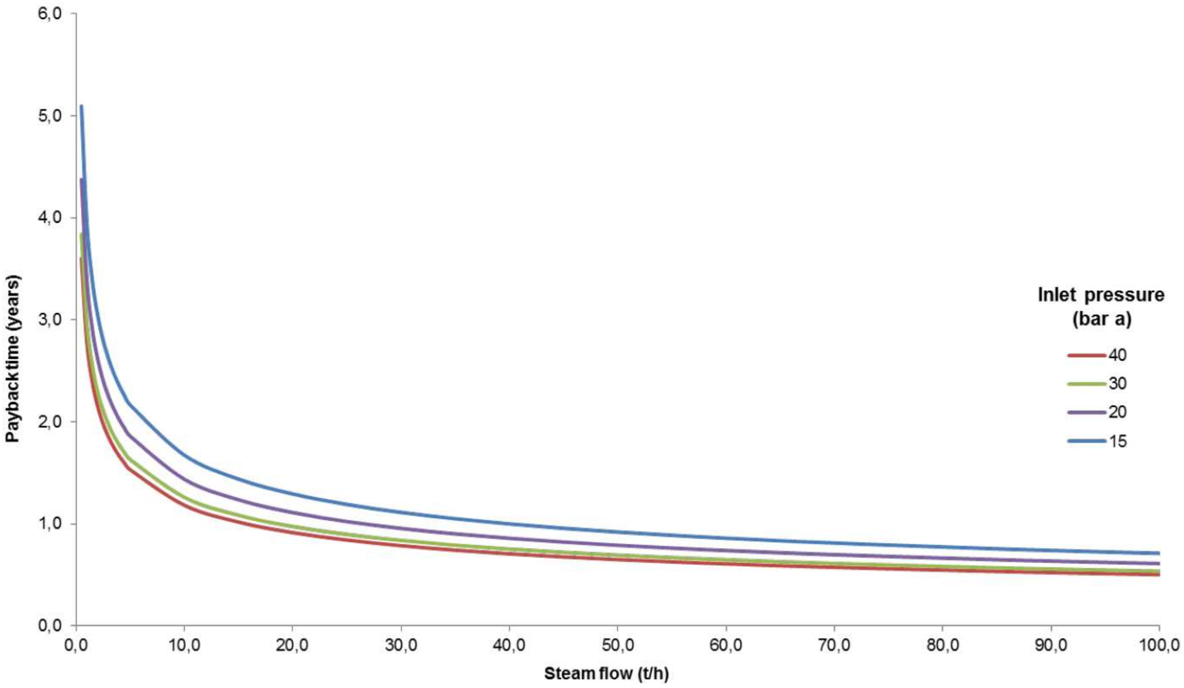
When applicable, the costs of power and steam were used from Table 3.2, realistic figures for the Brazilian market.

Sensitivity 1 - Payback time versus steam flow rate.

An analysis of the payback time (in comparison to valve throttling) sensibility in respect to steam flow rate was made.

The results, based on the case listed on Table 4.6 is shown on Figure 4.13.

Figure 4.13: Payback time versus steam flow rate



It is observable from the Figure 4.13 that payback time and consequently the attractiveness of installation of a steam turboexpander instead a valve have a flat, almost constant, behavior for higher steam flow. On the other hand is becomes quickly economically unfeasible for lower steam flow rates.

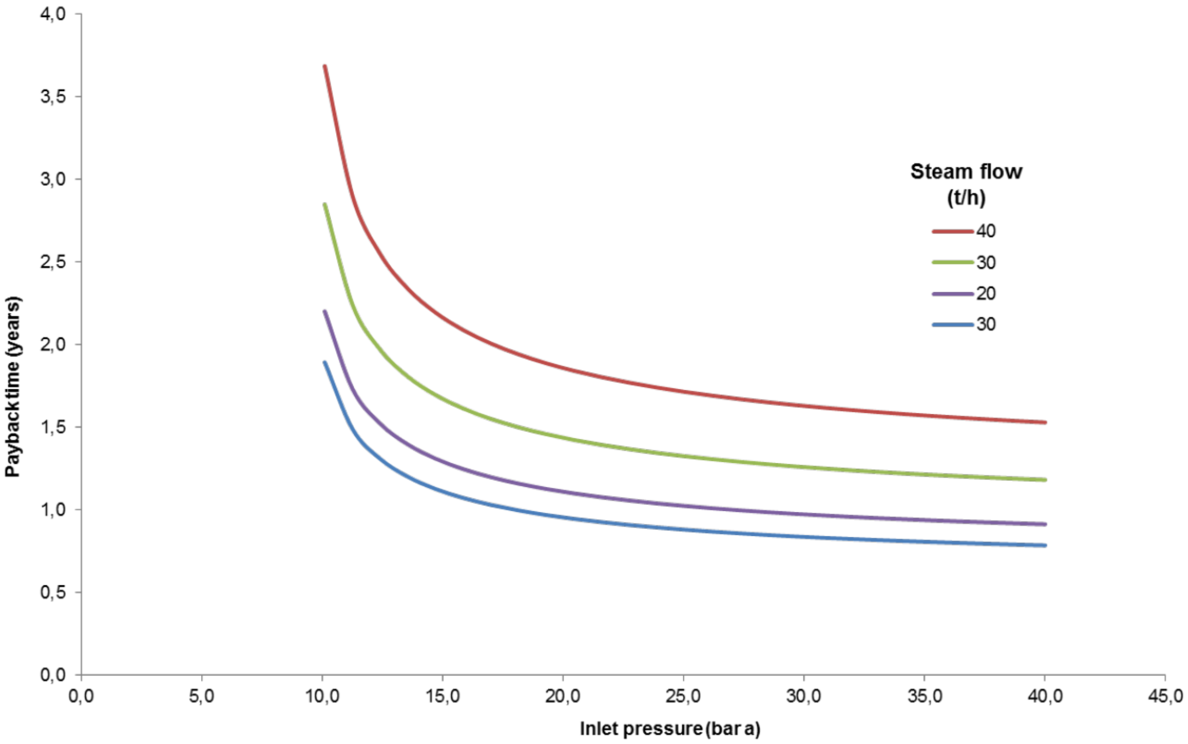
The attractiveness is almost insensitive to the developed pressure reduction on the steam turbine. This behavior will be investigated with more details on Sensitivity 2.

Sensitivity 2 - Payback time versus inlet pressure.

An analysis of the of payback time (in comparison to valve throttling) sensibility in respect to steam inlet pressure was made.

The results, based on the case shown on Table 4.6 is shown on Figure 4.14.

Figure 4.14: Payback time versus inlet pressure



The previous observation gets clearer here. The payback time is almost insensitive to inlet pressure from 20 bara onward, for a given flow rate.

Again, for low pressure reductions (and consequently lower useful work), the inlet pressure becomes important and the payback tend to infinity close to the outlet pressure.

Conclusion

Excepting the numeric values, it is expected that the analysis made and the observed behavior are valid for any steam turboexpansion scenario.

Expansion in turbine is heavily dependent on steam mass flow, showing itself economically feasible for higher mass flows, mainly due to increasing efficiencies.

New high efficiency micro-turbines can make it feasible for lower steam flows (see CARRIER and SPIRAX-SARCO in References).

4.5.3 Steam thermocompressor

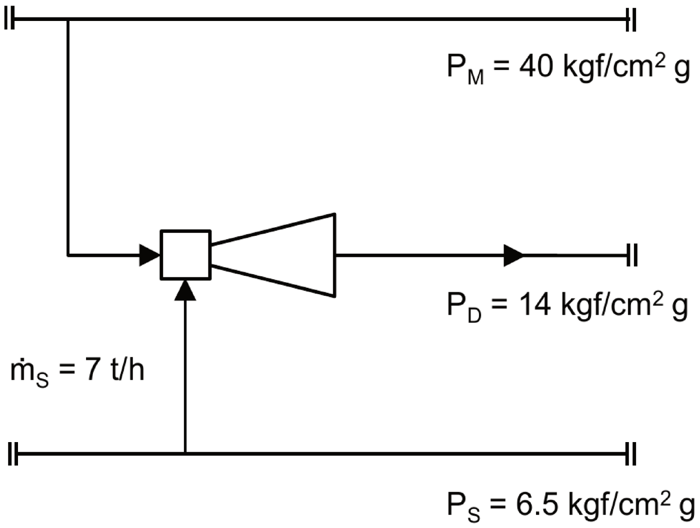
Base case

Table 4.7 shows the base case data used for the analysis presented here and Figure 4.15 illustrates the analyzed processes of steam thermocompression driven by a ejector.

Table 4.7: Steam thermocompression - base case conditions

Parameter	Value
Motive pressure (HP)	$40\,\mathrm{kgf/cm^2}$
Discharge pressure (MP)	$14\,\mathrm{kgf/cm^2}$
Suction pressure (LP)	$6.5\,\mathrm{kgf/cm^2}$
Suction flow rate ($\dot{m}_S$)	$7\,\mathrm{t/h}$

Figure 4.15: Base case schematics



These values were chosen based on typical pressure levels available on industrial steam networks.

Sensitivity analysis

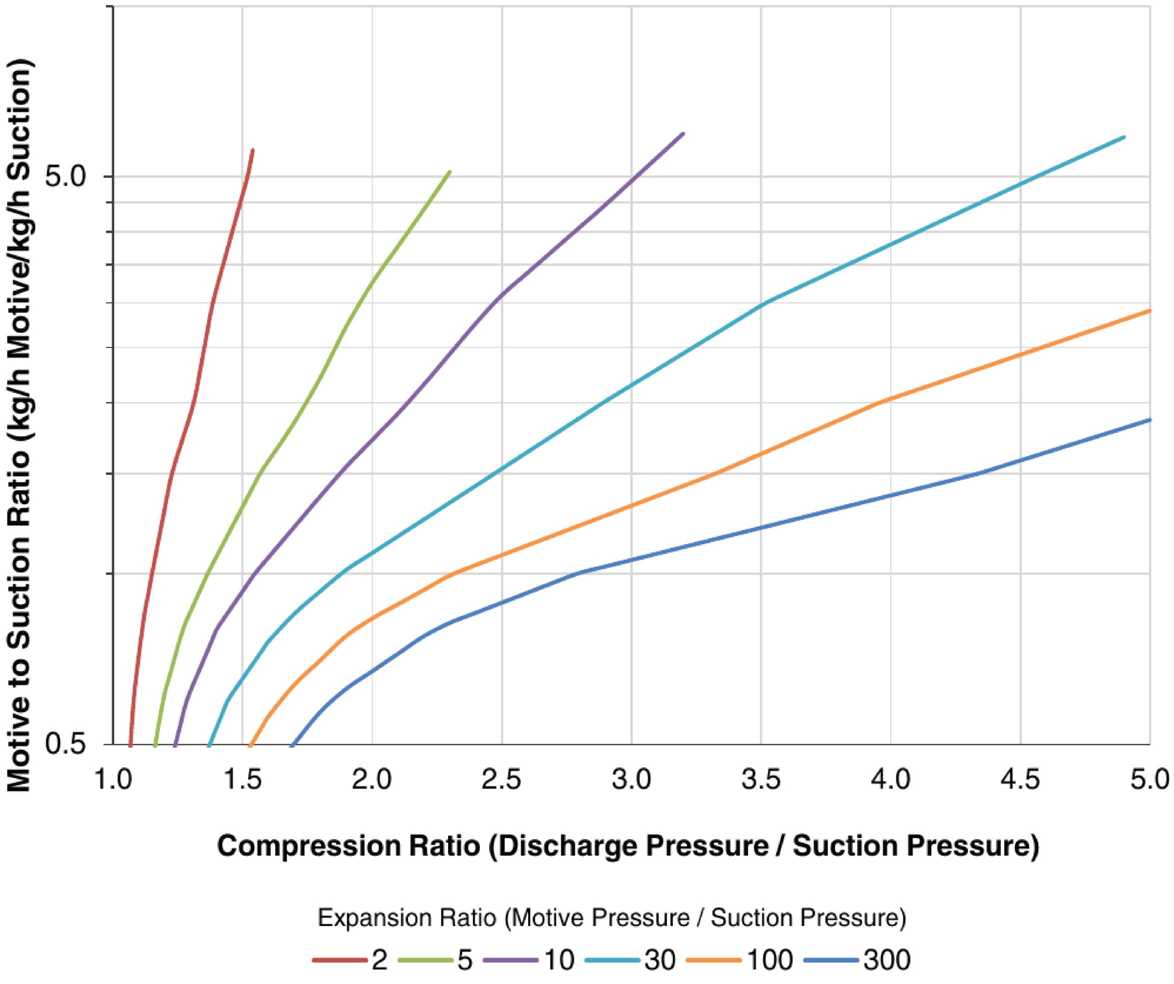
Three sensitivity analyses were constructed in order to assess the expected ejector performance under different process conditions. The focus is to get the frontiers of feasibility (technical and economic).

From now on, the performance of the thermocompression process will be assessed through the ratio between required motive steam and suction steam (motive to suction ratio).

Sensitivity 1 - Thermocompression performance versus Compression Ratio (CR)

Figure 4.16 shows the generalized performances curves in respect to Compression Ratio (CR) evaluated for some isoparametric curves of Expansion Ratios (ER).

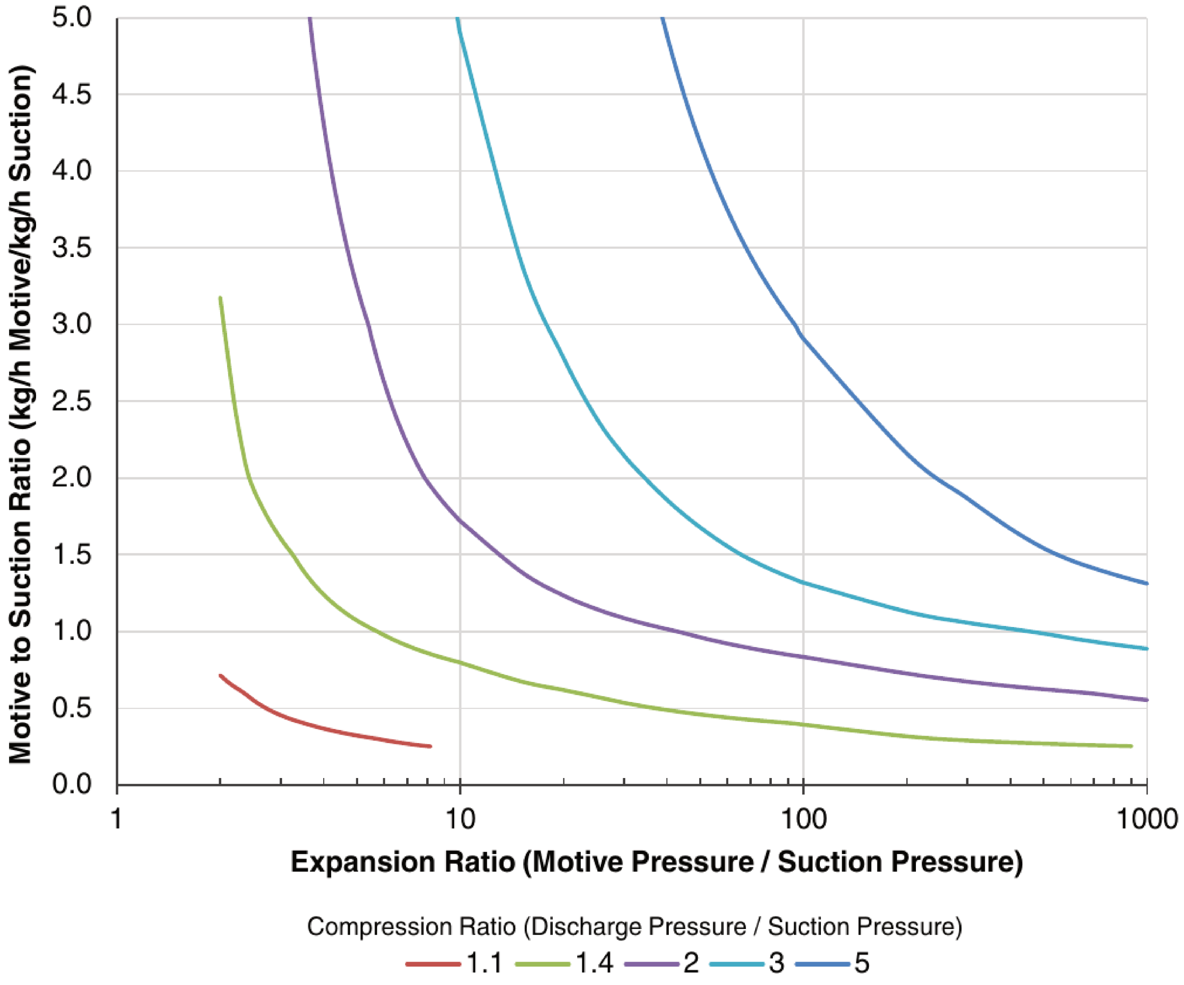
Figure 4.16: Generalized performance curves for each expansion ratio (ER)



Sensitivity 2 - Thermocompression performance versus Expansion Ratio (ER)

Figure 4.17 shows the generalized performance curves in respect to Expansion Ratio (ER) evaluated for some isoparametric curves of Compression Ratios (CR).

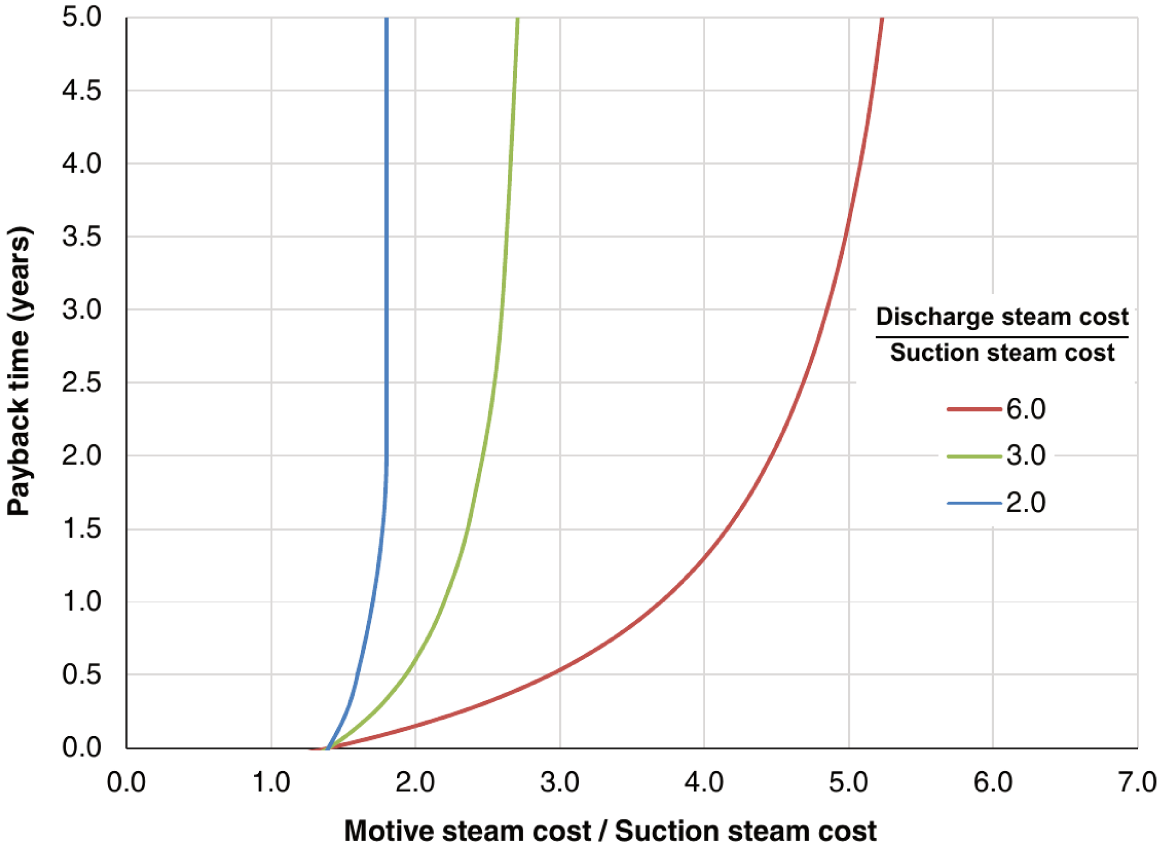
Figure 4.17: Generalized performance curves for each compression ratio (CR)



Sensitivity 3 - Payback time versus ratio between costs of motive and suction steam

Figure 4.18 presents the economic feasibility frontiers for 3 different cost ratio between discharge steam (intermediate pressure) and suction steam (lower pressure), in respect to cost ratio between motive (higher pressure) steam and suction steam.

Figure 4.18: Simple payback curves for 3 different cost ratios



Conclusion

Economic feasibility depends heavily on cost of steam levels and/or opportunity costs on utilizing HP steam to produce work on a turbine.

It can be inferred that, for a more realistic scenario where motive steam is considerably more expensive than steam at suction pressure, attractive simple payback times are only achievable if steam at discharge pressure is as valuable as motive steam or steam at suction pressure is close to null cost. This behavior is strengthened because thermocompression efficiency is higher at low CR and at low driving pressures ratio.

4.6 Utilities systems

4.6.1 Thermal insulation

Base case

The results shown here are based on the base case described on Tables 4.8 and 4.9, for the hot and cold cases, respectively.

Table 4.8: Thermal insulation - base case conditions (hot case)

Parameter	**Value**
Ambient temperature (T_∞)	$25\,^\circ\mathrm{C}$
Bare surface temperature (T_S)	$250\,^\circ\mathrm{C}$
Mean air speed (v_∞)	$5\,\mathrm{km/h}$
Insulation material	Calcium silicate

Table 4.9: Thermal insulation - base case conditions (cold case)

Parameter	**Value**
Ambient temperature (T_∞)	$25\,^\circ\mathrm{C}$
Bare surface temperature (T_S)	$5\,^\circ\mathrm{C}$
Mean solar irradiance (I_sun)	$400\,\mathrm{W/m^2}$
Daylight hours (DLH)	$12\,\mathrm{h/day}$
Mean air speed (v_∞)	$5\,\mathrm{km/h}$
Insulation material	PU foam

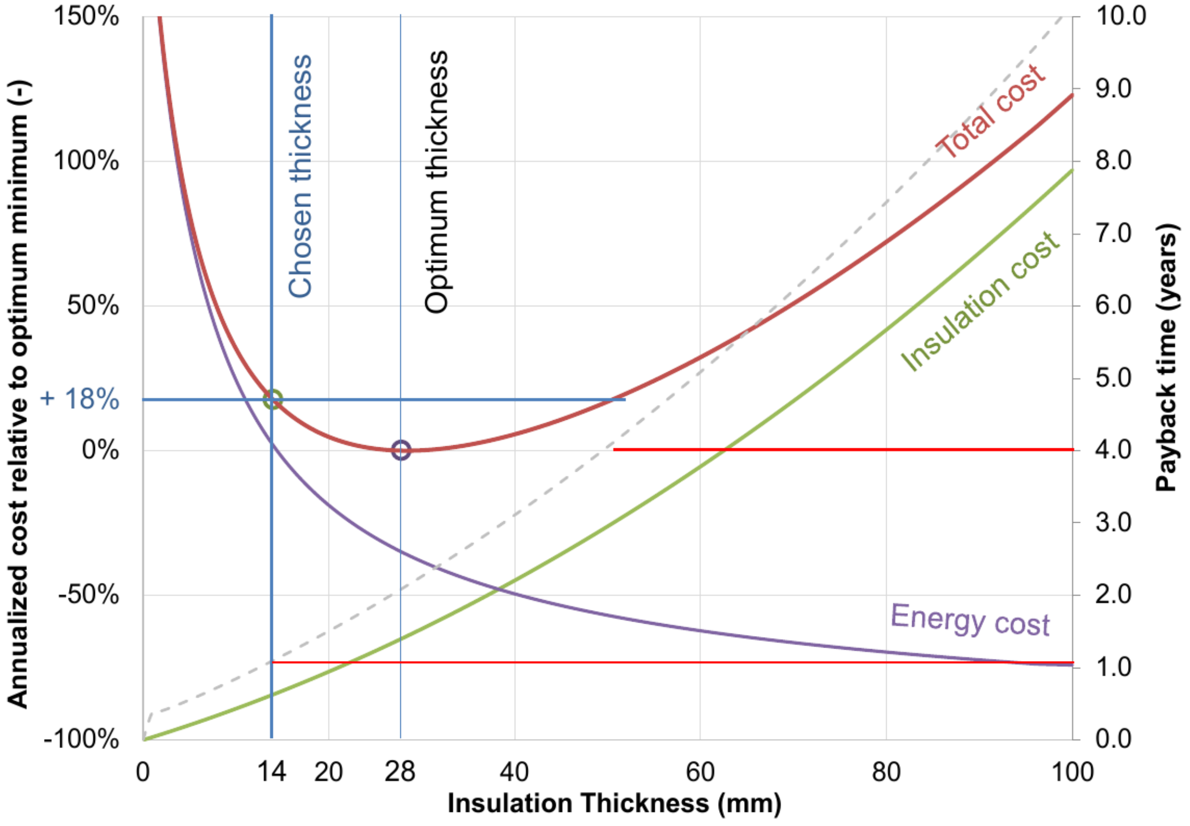
The values assumed on Tables 4.8 and 4.9 are realistic figures for hot streams, such as medium pressure superheated steam (10 - 40 barg). Calcium Silicate is a common insulation material used in the industry due its cost and ease of installation. The assumed value for mean air speed is typical of light breezes, according to the Beaufort scale.

Polyurethane foam is commonly used to insulating cold surfaces. The mean solar irradiance assumed is a fair value, typical for low to middle latitude locations.

Sensitivity 1 - Total cost versus insulation thickness

The total cost curve of an installed insulation in respect to the chosen insulation thickness is shown on Figure 4.19.

Figure 4.19: Total cost of an insulated setup

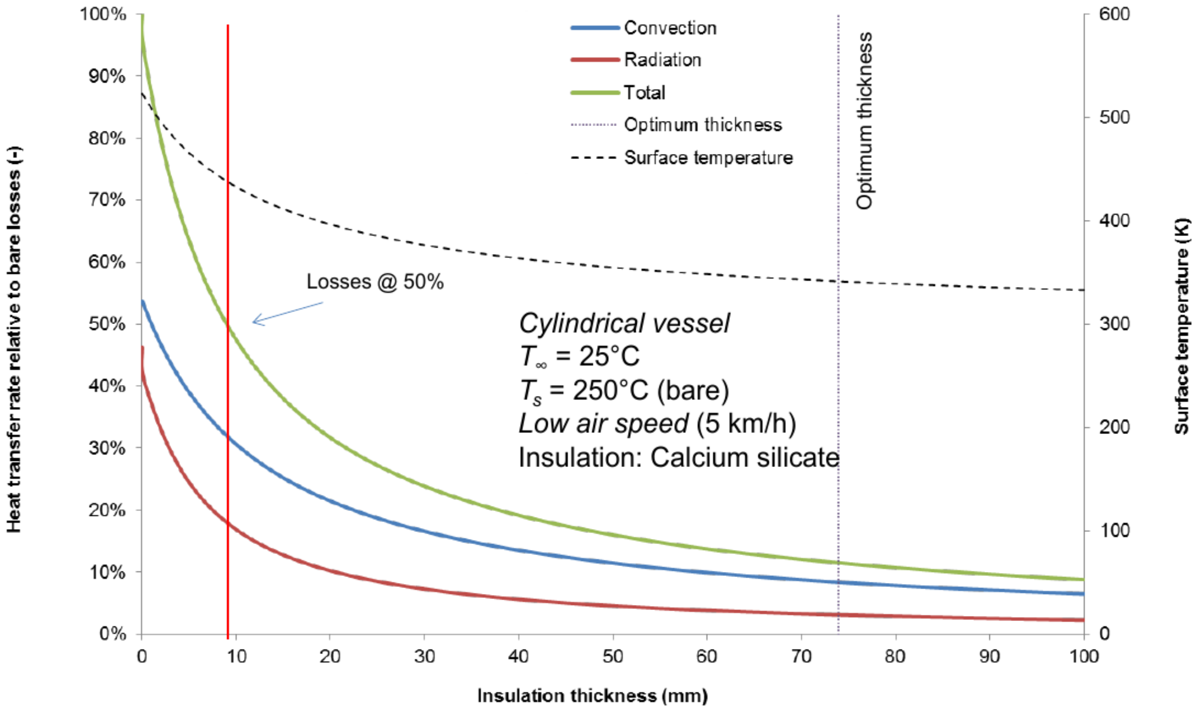


Sensitivity 2 - Heat transfer rate versus insulation thickness

Heat transfer rate sensitivity studies were performed as a function of the insulation thickness, from the base cases shown on Tables 4.8 and 4.9.

Figure 4.20 shows the components of heat losses from a heated surface (a piping, tank or other equipment), varying in respect to insulation thickness.

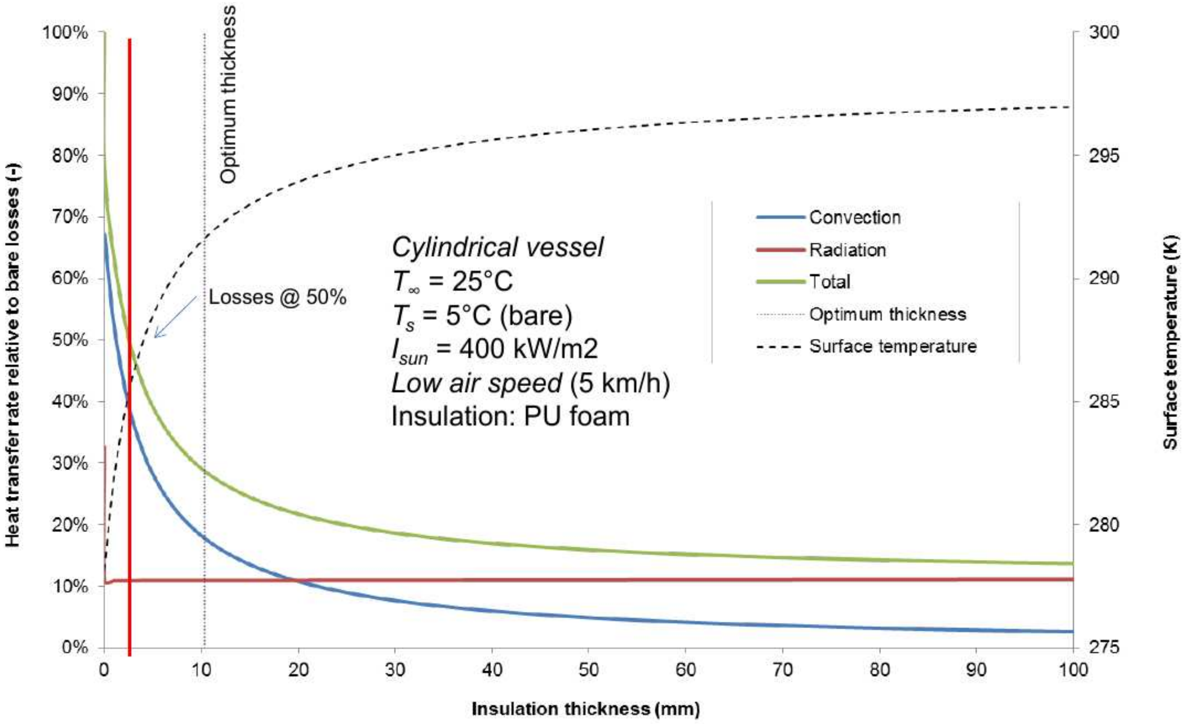
Figure 4.20: Breakdown of losses (hot case)



It is interesting to note that an insulation of only 10 mm provides a reduction of half when compared to a bare surface, while the optimum calculated insulation thickness is 73 mm.

Conversely, the Figure 4.21 shows the components of heat “gains” to a cold surface (a piping, tank or other equipment).

Figure 4.21: Breakdown of losses (cold case)



It is possible to note, from Figure 4.21, that just the reduction on the solar absorptance have a significant effect on reducing the total heating. This can be accomplished by metallic protection of insulation or painting with light colors.

Comparing Figures 4.20 and 4.21 to Figure 4.19, it can be seen that further increasing insulation thickness after some point can be worthless.

Conclusion

In general, caution must be taken when evaluating thermal insulation investment based on rules of thumb and previously calculated economic thicknesses, especially regarding processes and installations on which heat insulation become a important share of total investment (mainly extreme hot or cold processes).

Many projects of revamp or new thermal insulation for heat conservation can show itself little attractive when evaluated near optimum thickness, but a way thinner (and cheaper) insulation can drive a considerable amount of the targeted savings.

Chapter 5

General conclusion

This final chapter reviews briefly general conclusions and presents some suggestions for future work. Specific conclusions of each topic were addressed at the end of the sections on Chapter 4.

As proposed, simplified models and tools for 7 systems were developed, with the purpose of assist and contribute to quick assessment of alternatives.

Each section of “Results and discussion” bring some conclusion and a sensitivity on how to quickly assess the associated costs and savings regarding the studied topics.

The tools developed present a consistent interface and their inputs and outputs are as similar as possible. The main screen of each spreadsheet is shown on Appendix B.

This work must be viewed as a initial and a modest contribution to process synthesis, regarding each one of the fields of process design: reaction, separation, thermal exchange and utility allocation, besides the moment transfer operations that permeate all these fields.

These contributions can help to fill some gaps not addressed in existing literature, regarding early stage process design, and can be used on manual or automated procedures of synthesis and decision to get quicker screening studies.

This work is evolutive and the same structure presented here can be used on other systems and under different conditions. The same approach adopted in this work can be applied to other systems, reinforcing the importance of constructing fields of sensitivity and feasibility.

5.1 Suggestions for future work

Some tools are under development for future publication. The subjects are listed on Table 5.1.

Table 5.1: Subjects under development, grouped by onion layers (and slice)

Layer	No.	Short description
S	2.2	Side reboilers
HEN	3.2	Heat Exchanger Fouling
MTO	4.5	Gas turboexpansion
	4.6	Energy Recovery Devices
	4.7	Vacuum systems
U	5.2	Cooling water system assessment
	5.3	Chiller technologies assessment
	5.4	Refrigeration systems
	5.5	Steam leaks
	5.6	Variable Speed Driver
	5.7	Electric motors replacement
	5.8	Organic Rankine Cycle feasiblity

Besides that, some improvements on the presented subjects can be carried out as suggested below.

Heat pump assisted distillation

For the MVC distillation, the analysis should be improved in order to conciliate systems where the total pumped heat is not enough to supply all the duty required to the reboiler.

Steam turboexpansion

The sensitivity should be updated with the newer microturbines attainable efficiencies.

5.2 General references

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Appendix A

Data tables

A.2.1 Specific energy consumption in chemical processes

Data table

Table A.1: Data collection, reported SEC, estimated SEC and relative deviation

#	**Product**	ΔH_R	**SEC**	**SEC'- SEC**	$\frac{\text{SEC'-SEC}}{\sigma}$	**Ref**
			(MJ/kg$_{\text{prod}}$)			
1	1,4-Butanediol	-4.8	25.4	-20.2	2.2	[5]
2	1-Propanol	-1.1	2.6	6.3	0.7	[5]
3	2-Butanol	-0.6	30.8	-21.2	2.3	[5]
4	2-Propenenitrile	-11.3	3.7	-5.0	0.5	[5]
5	Acetaldehyde	-5.0	5.2	-0.2	0.0	[2]
6	Acetaldehyde	-5.0	3.5	1.5	0.2	[2]
7	Acetaldehyde	-5.0	3.4	1.6	0.2	[2]
8	Acetic acid	-4.8	1.9	3.3	0.4	[3]
9	Acetic acid	-1.8	6.7	1.2	0.1	[3]
10	Acetic Acid	*1.0 **	5.9	6.8	0.8	[7]
11	Acetic Anhydride	*-4.8 **	6.5	-1.2	0.1	[7]
12	Acetic anhydride - product	-0.5	19.4	-9.6	1.1	[5]
13	Acetone	*-2.7 **	17.9	-10.6	1.2	[7]
14	Acrylic Acid	*-4.2 **	21.0	-15.1	1.7	[7]
15	Acrylonitrile	-10.3	2.6	-2.9	0.3	[3]
16	Acrylonitrile	*-12.8 **	1.5	-4.3	0.5	[7]
17	Adhesives and sealants	0.0	3.0	7.7	0.8	[2]
18	Adipic acid	-7.2	33.0	-30.2	3.3	[3]
19	Aluminum sulfate	-0.7	5.6	3.9	0.4	[2]
20	Aluminum Sulfate	*-0.4 **	2.9	7.1	0.8	[7]
21	Ammonia	*1.0 **	13.6	-0.9	0.1	[7]
22	Ammonium nitrate	-1.8	5.1	2.8	0.3	[2]
23	Ammonium Nitrate	*-1.2 **	0.8	8.0	0.9	[7]

(cont.)

	Product	ΔH_R	**SEC**	**SEC'- SEC**	$\frac{\text{SEC'-SEC}}{\sigma}$	**Ref**
			(MJ/kg$_{prod}$)			
24	Ammonium Phosphates (Other)	_-0.6 *_	0.8	9.0	1.0	[7]
25	Ammonium Sulfate	_-1.6 *_	9.3	-1.2	0.1	[7]
26	Aniline	_-4.9 *_	-2.3	7.4	0.8	[7]
27	Benzene	0.0	12.5	-1.8	0.2	[3]
28	Benzene	-0.5	1.0	8.8	1.0	[3]
29	Benzene	-0.6	2.6	7.1	0.8	[5]
30	Benzene	_-0.2 *_	18.3	-7.9	0.9	[7]
31	Benzyl alcohol	0.7	4.4	7.6	0.8	[5]
32	Bisphenol A	_-1.1 *_	21.9	-13.1	1.4	[7]
33	Bisphenol A	-0.3	18.2	-8.1	0.9	[2]
34	Bisphenol A	-0.3	16.6	-6.5	0.7	[2]
35	Butadiene	0.0	9.1	1.6	0.2	[3]
36	Butadiene	_-1.2 *_	18.3	-9.5	1.1	[7]
37	Butylenes	_-1.2 *_	3.9	4.9	0.5	[7]
38	Calcium Carbonate	_0.2 *_	4.8	6.4	0.7	[7]
39	Calcium Chloride	_-5.7 *_	9.0	-4.8	0.5	[7]
40	Caprolactam	-9.3	45.6	-44.9	5.0	[3]
41	Caprolactam	_-0.9 *_	30.7	-21.4	2.4	[7]
42	Carbon Black	_-1.9 *_	8.9	-1.1	0.1	[7]
43	Carbon Dioxide	_-9.0 *_	0.7	0.3	0.0	[7]
44	Chlorine	-1.4	0.2	8.2	0.9	[2]
45	Chlorine	6.4	30.7	4.5	0.5	[3]
46	Chlorine	6.4	28.5	6.8	0.7	[3]
47	Chlorine	6.4	24.4	10.9	1.2	[3]
48	Chlorine	_7.2 *_	15.3	25.7	2.8	[7]
49	Chlorine (and caustic soda)	6.3	42.5	-8.0	0.9	[2]
50	Chlorine (and caustic soda)	6.3	39.5	-5.0	0.6	[2]
51	Chlorobenzene	-1.3	1.4	7.2	0.8	[5]
52	Cumene	-0.9	2.1	7.1	0.8	[3]
53	Cyclohexane	-2.4	0.0	7.2	0.8	[2]
54	Cyclohexane	-2.4	2.8	4.4	0.5	[2]
55	Cyclohexane	-2.4	-1.2	8.4	0.9	[3]
56	Cyclohexane	-2.4	4.0	3.1	0.3	[5]
57	Cyclohexane	_-5.5 *_	-1.3	5.8	0.6	[7]
58	Cyclohexanone	-3.8	21.7	-15.5	1.7	[5]
59	Cyclohexanone	_-13.7 *_	0.2	-3.9	0.4	[7]
60	Diammonium Phosphate	_-0.6 *_	0.8	9.0	1.0	[7]
61	Dimethyl terephthalate	0.1	14.5	-3.7	0.4	[2]
62	Dimethyl terephthalate	0.1	11.9	-1.1	0.1	[2]
63	Dimethylterephtalate	-6.1	5.9	-2.0	0.2	[3]
64	Ethanol	-1.0	14.6	-5.5	0.6	[2]
65	Ethanol	-1.0	12.4	-3.3	0.4	[2]
66	Ethanol	-1.0	2.8	6.2	0.7	[5]

(cont.)

	Product	**ΔH_R**	**SEC**	**SEC'- SEC**	**$\frac{\text{SEC'-SEC}}{\sigma}$**	**Ref**
			(MJ/kg$_{prod}$)			
67	Ethanol	_-3.8 *_	10.8	-4.6	0.5	[7]
68	Ethyl acetate	-1.7	4.2	3.9	0.4	[2]
69	Ethyl benzene	-1.1	0.1	8.8	1.0	[2]
70	Ethylbenzene	-1.1	-0.8	9.7	1.1	[3]
71	Ethylbenzene	_0.6 *_	2.7	9.2	1.0	[7]
72	Ethylene	6.7	35.5	1.7	0.2	[3]
73	Ethylene	4.1	24.1	-1.7	0.2	[3]
74	Ethylene	4.6	22.0	2.9	0.3	[3]
75	Ethylene	5.4	23.5	5.5	0.6	[3]
76	Ethylene	_2.3 *_	16.4	-0.3	0.0	[7]
77	Ethylene Dichloride	_-1.8 *_	7.9	0.0	0.0	[7]
78	Ethylene glycol	-2.7	6.4	1.0	0.1	[3]
79	Ethylene Glycol	_-1.0 *_	4.8	4.3	0.5	[7]
80	Ethylene oxide	-2.3	7.0	0.2	0.0	[2]
81	Ethylene oxide	-2.3	-1.5	8.8	1.0	[2]
82	Ethylene oxide	-2.4	5.7	1.5	0.2	[3]
83	Ethylene Oxide	_1.7 *_	4.5	10.0	1.1	[7]
84	Formaldehyde	-5.4	-0.9	5.5	0.6	[2]
85	Formaldehyde	-5.4	-4.0	8.6	0.9	[2]
86	Formaldehyde	-5.4	-4.4	9.0	1.0	[2]
87	Formaldehyde	-5.4	-4.3	8.8	1.0	[2]
88	Formaldehyde	-3.7	-3.6	9.9	1.1	[3]
89	Formic acid - product	0.5	19.7	-7.9	0.9	[5]
90	Hydrochloric Acid	_-2.6 *_	0.4	7.0	0.8	[7]
91	Hydrogen	_-11.3 *_	2.2	-3.5	0.4	[7]
92	Hydrogen fluoride	1.4	16.8	-3.1	0.3	[2]
93	Hydrogen fluorisde	1.4	15.5	-1.8	0.2	[2]
94	Hydrogen Peroxide	_-3.6 *_	16.2	-9.8	1.1	[7]
95	Isobutylene	_0.1 *_	7.6	3.3	0.4	[7]
96	Isopropanol	-0.9	19.0	-9.8	1.1	[2]
97	Isopropanol	-0.9	10.3	-1.1	0.1	[2]
98	Isopropanol	_-0.1 *_	10.9	-0.4	0.0	[7]
99	Maleic anhydride	-19.2	-13.6	4.5	0.5	[2]
100	Maleic anhydride	-19.2	-17.8	8.6	1.0	[2]
101	Methanol	0.0	19.2	-8.5	0.9	[3]
102	Methanol	_1.9 *_	11.4	3.5	0.4	[7]
103	Methyl acrylate	-1.1	14.9	-6.0	0.7	[2]
104	Methyl Chloride	_-0.6 *_	2.0	7.7	0.9	[7]
105	Methyl Methacrylate	_-14.8 *_	8.1	-12.9	1.4	[7]
106	Methyl tert butyl ether	-0.7	4.4	5.2	0.6	[3]
107	Methyl tert-Butyl Ether	_0.3 *_	4.4	6.9	0.8	[7]
108	MIBK	-1.0	7.0	2.0	0.2	[5]
109	Monoammonium Phosphate	_-0.6 *_	0.8	9.0	1.0	[7]

(cont.)

	Product	ΔH_R	**SEC**	**SEC'- SEC**	$\frac{\text{SEC'-SEC}}{\sigma}$	**Ref**
		(MJ/kg$_{\text{prod}}$)				
110	Nitric acid	-7.1	-1.3	4.2	0.5	[2]
111	Nitrobenzene	_-0.7 *_	1.3	8.2	0.9	[7]
112	Nitrogen	_0.0 *_	1.8	8.9	1.0	[7]
113	n-Paraffins	0.0	6.7	4.0	0.4	[2]
114	Oxygen	0.0	7.7	3.0	0.3	[2]
115	Oxygen	0.0	3.4	7.3	0.8	[2]
116	Oxygen	_0.0 *_	1.8	8.9	1.0	[7]
117	PET	0.2	5.9	5.1	0.6	[3]
118	Phenol	_-8.3 *_	8.5	-6.8	0.8	[7]
119	Phenol / acetone	-3.8	12.1	-5.9	0.7	[3]
120	Phithalic anhydride	-8.0	2.3	-0.3	0.0	[3]
121	Phosphoric Acid	_-0.9 *_	1.1	8.0	0.9	[7]
122	Phtalic anhydride	-8.0	2.3	-0.3	0.0	[3]
123	Phtalic anhydride	-12.5	-8.4	5.9	0.6	[3]
124	Polycarbonate	_0.1 *_	15.6	-4.7	0.5	[7]
125	Polyester	_-2.4 *_	28.2	-21.0	2.3	[7]
126	Polyetherpolyols	0.0	1.7	9.0	1.0	[3]
127	Polyethylene	-3.8	5.2	0.9	0.1	[3]
128	Polyethylene (high-density)	-3.4	9.2	-2.6	0.3	[2]
129	Polyethylene (high-density)	-3.4	4.4	2.2	0.2	[2]
130	Polyethylene (high-density)	-3.4	4.7	1.9	0.2	[2]
131	Polyethylene (high-density)	-3.4	0.9	5.7	0.6	[2]
132	Polyethylene (low-density)	-3.4	5.5	1.1	0.1	[2]
133	Polyethylene (low-density)	-3.4	8.3	-1.6	0.2	[2]
134	Polyethylene High Density	_-4.1 *_	2.4	3.5	0.4	[7]
135	Polyethylene Linear Low Density	_-2.6 *_	2.0	5.4	0.6	[7]
136	Polyethylene Low Density	_-4.1 *_	2.7	3.3	0.4	[7]
137	Polyethylene Terephthalate	_-2.4 *_	5.3	1.8	0.2	[7]
138	Polypropylene	-2.0	6.8	0.8	0.1	[2]
139	Polypropylene	-2.0	9.9	-2.3	0.3	[2]
140	Polypropylene	-2.5	3.5	3.7	0.4	[3]
141	Polypropylene	_-2.7 *_	1.4	5.9	0.6	[7]
142	Polystyrene	-0.7	5.2	4.3	0.5	[2]
143	Polystyrene	-0.7	1.4	8.2	0.9	[3]
144	Polystyrene	_-1.1 *_	5.3	3.6	0.4	[7]
145	Polystyrene High Impact	_-1.1 *_	1.5	7.4	0.8	[7]
146	Polyurethane	0.0	3.3	7.4	0.8	[3]
147	Polyurethane	0.0	3.3	7.4	0.8	[3]
148	Polyurethane	_0.4 *_	0.3	11.2	1.2	[7]
149	Polyvinyl chloride	-1.5	14.0	-5.7	0.6	[2]
150	Polyvinyl chloride	-1.5	3.2	5.1	0.6	[2]
151	Polyvinyl chloride	-1.5	1.6	6.6	0.7	[2]
152	Polyvinyl Chloride	_-2.3 *_	3.4	4.0	0.4	[7]

(cont.)

	Product	ΔH_R	**SEC**	**SEC'- SEC**	$\frac{\text{SEC'-SEC}}{\sigma}$	**Ref**
			(MJ/kg$_{\text{prod}}$)			
153	Potassium chloride	0.0	3.6	7.1	0.8	[2]
154	Potassium hydroxide	4.0	26.3	-4.2	0.5	[2]
155	Printing inks	0.0	3.5	7.2	0.8	[2]
156	Propylene	*2.0* *	3.1	12.0	1.3	[7]
157	Propylene oxide	-3.8	15.4	-9.2	1.0	[3]
158	Propylene Oxide	*0.1* *	6.0	5.0	0.5	[7]
159	PVC	-2.1	3.3	4.3	0.5	[3]
160	p-Xylene	0.0	3.9	6.8	0.8	[2]
161	p-xylene	0.0	10.3	0.4	0.0	[3]
162	sec-Butyl alcohol	-0.8	12.2	-2.8	0.3	[2]
163	sec-Butyl alcohol	-0.8	12.4	-3.0	0.3	[2]
164	Soda Ash	*-4.1* *	6.9	-1.0	0.1	[7]
165	Sodium carbonate	0.1	15.1	-4.2	0.5	[2]
166	Sodium Hydroxide	*-7.8* *	8.8	-6.5	0.7	[7]
167	Sodium Hypochlorite	*-0.1* *	1.4	9.2	1.0	[7]
168	Sodium silicate	0.6	7.2	4.8	0.5	[2]
169	Sodium silicate	0.6	11.6	0.3	0.0	[2]
170	Sodium Silicates	*-12.0* *	5.3	-7.4	0.8	[7]
171	Sodium sulfate	0.0	6.0	4.8	0.5	[2]
172	Styrene	0.0	16.3	-5.6	0.6	[2]
173	Styrene	0.0	11.3	-0.5	0.1	[2]
174	Styrene	1.1	9.1	4.0	0.4	[3]
175	Styrene	*0.8* *	8.8	3.5	0.4	[7]
176	Sulfuric Acid	*-6.7* *	-2.1	5.3	0.6	[7]
177	Terephthalic acid	-7.6	7.2	-4.8	0.5	[3]
178	Terephthalic Acid	*-6.8* *	5.2	-2.0	0.2	[7]
179	Trichlorofluoro-methane	0.2	3.5	7.6	0.8	[2]
180	Urea	-2.2	3.1	4.3	0.5	[2]
181	Urea	-2.2	2.7	4.7	0.5	[2]
182	Urea	0.0	2.4	8.3	0.9	[3]
183	Urea	*-0.7* *	2.0	7.6	0.8	[7]
184	Vinyl Acetate	*-2.5* *	8.4	-1.3	0.1	[7]
185	Vinyl Chloride	*0.3* *	4.9	6.4	0.7	[7]
186	Vinylchloride	-2.3	5.8	1.5	0.2	[3]
187	Xylenes Mixed	*-0.8* *	2.9	6.5	0.7	[7]
188	Xylenes Paraxylene	*0.0* *	5.9	4.8	0.5	[7]
189	N/A	-2.3	4.3	2.9	0.3	[4]
190	N/A	-2.3	17.1	-9.8	1.1	[4]
191	N/A	-0.4	7.0	3.0	0.3	[4]
192	N/A	-2.7	10.1	-2.8	0.3	[4]
193	N/A	0.0	7.6	3.1	0.3	[4]
194	N/A	0.0	17.1	-6.4	0.7	[4]
195	N/A	-0.7	24.1	-14.7	1.6	[4]

(cont.)

	Product	ΔH_R	**SEC**	**SEC'- SEC**	$\frac{\text{SEC'-SEC}}{\sigma}$	**Ref**
		(MJ/kg$_{prod}$)				
196	N/A	0.0	24.8	-14.1	1.6	[4]
197	N/A	0.0	3.6	7.1	0.8	[4]
198	N/A	-0.7	26.6	-17.2	1.9	[4]
199	N/A	-0.2	2.2	8.2	0.9	[4]
200	N/A	-0.2	2.7	7.7	0.8	[4]
201	N/A	0.0	3.2	7.5	0.8	[4]
202	N/A	-0.2	2.7	7.6	0.8	[4]
203	N/A	0.0	6.8	3.9	0.4	[4]
204	N/A	1.2	15.1	-2.0	0.2	[6]
205	N/A	1.2	10.2	2.9	0.3	[6]
206	N/A	0.9	8.7	3.8	0.4	[6]
207	N/A	0.9	14.5	-2.0	0.2	[6]
208	N/A	-0.1	1.7	8.9	1.0	[6]
209	N/A	-0.2	5.7	4.7	0.5	[6]
210	N/A	-0.5	13.4	-3.5	0.4	[6]
211	N/A	-0.5	1.1	8.8	1.0	[6]
212	N/A	-0.9	10.7	-1.6	0.2	[6]
213	N/A	-0.8	4.9	4.5	0.5	[6]
214	N/A	-0.8	1.2	8.2	0.9	[6]
215	N/A	-0.9	10.1	-0.9	0.1	[6]
216	N/A	-1.1	15.2	-6.3	0.7	[6]
217	N/A	-1.0	4.3	4.7	0.5	[6]
218	N/A	-1.2	12.1	-3.4	0.4	[6]
219	N/A	-1.4	9.4	-0.9	0.1	[6]
220	N/A	-2.1	5.1	2.4	0.3	[6]
221	N/A	-2.3	7.8	-0.5	0.1	[6]
222	N/A	-2.4	-1.6	8.8	1.0	[6]
223	N/A	-2.4	5.0	2.2	0.2	[6]
224	N/A	-2.4	-2.0	9.2	1.0	[6]
225	N/A	-3.5	5.6	0.8	0.1	[6]
226	N/A	-4.0	4.2	1.8	0.2	[6]
227	N/A	-4.2	4.9	0.9	0.1	[6]
228	N/A	-5.4	4.0	0.7	0.1	[6]
229	N/A	-5.5	2.8	1.6	0.2	[6]
230	N/A	-5.6	4.4	0.0	0.0	[6]
231	N/A	-5.8	3.2	1.0	0.1	[6]
232	N/A	-7.5	-2.3	4.8	0.5	[6]
233	N/A	-8.2	8.9	-7.1	0.8	[6]
234	N/A	-9.7	3.0	-2.7	0.3	[6]
235	N/A	-9.7	2.0	-1.7	0.2	[6]
236	N/A	-12.1	-7.4	5.3	0.6	[6]
237	N/A	-12.7	-11.3	8.6	1.0	[6]
238	N/A	-15.0	-4.9	-0.1	0.0	[6]

Note: $\Delta X_{R\,=}\ \Delta H_R$ or ΔG_R. Figures indicated in italics and with * correspond to values of ΔG_R. Other values correspond to ΔH_R.

N/A - Product not disclosed by author.

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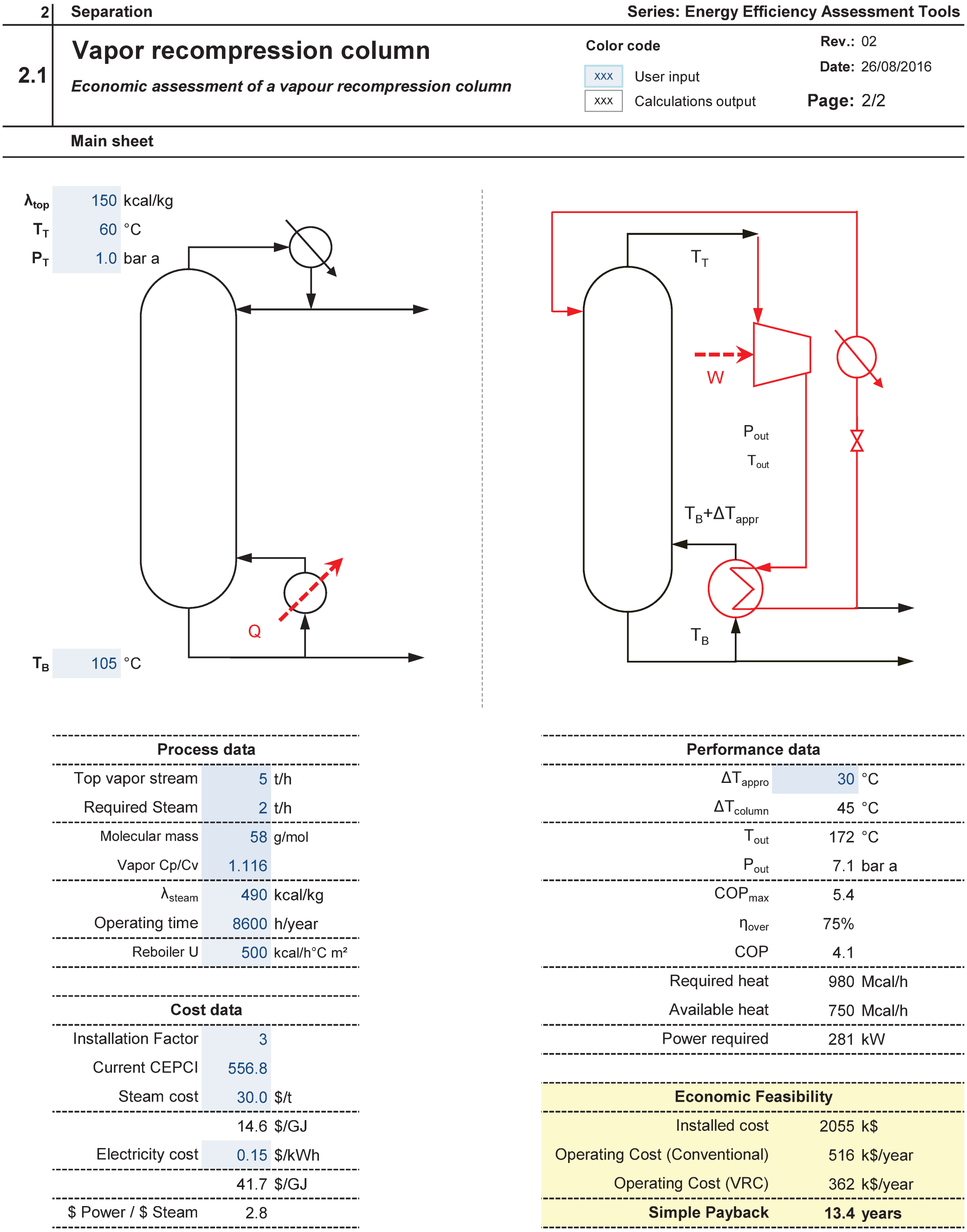
Appendix B

Tools screens

B.2 Separation operations

B.2.1 Heat pump assisted distillation



2 | **Separation** | **Series: Energy Efficiency Assessment Tools**

2.1

Vapor recompression column

Economic assessment of a vapour recompression column

Color code

xxx User input

xxx Calculations output

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Main sheet

λ_{top}	150	kcal/kg
T_T	60	°C
P_T	1.0	bar a
T_B	105	°C

Process data		
Top vapor stream	5	t/h
Required Steam	2	t/h
Molecular mass	58	g/mol
Vapor Cp/Cv	1.116	
λ_{steam}	490	kcal/kg
Operating time	8600	h/year
Reboiler U	500	kcal/h°C m²

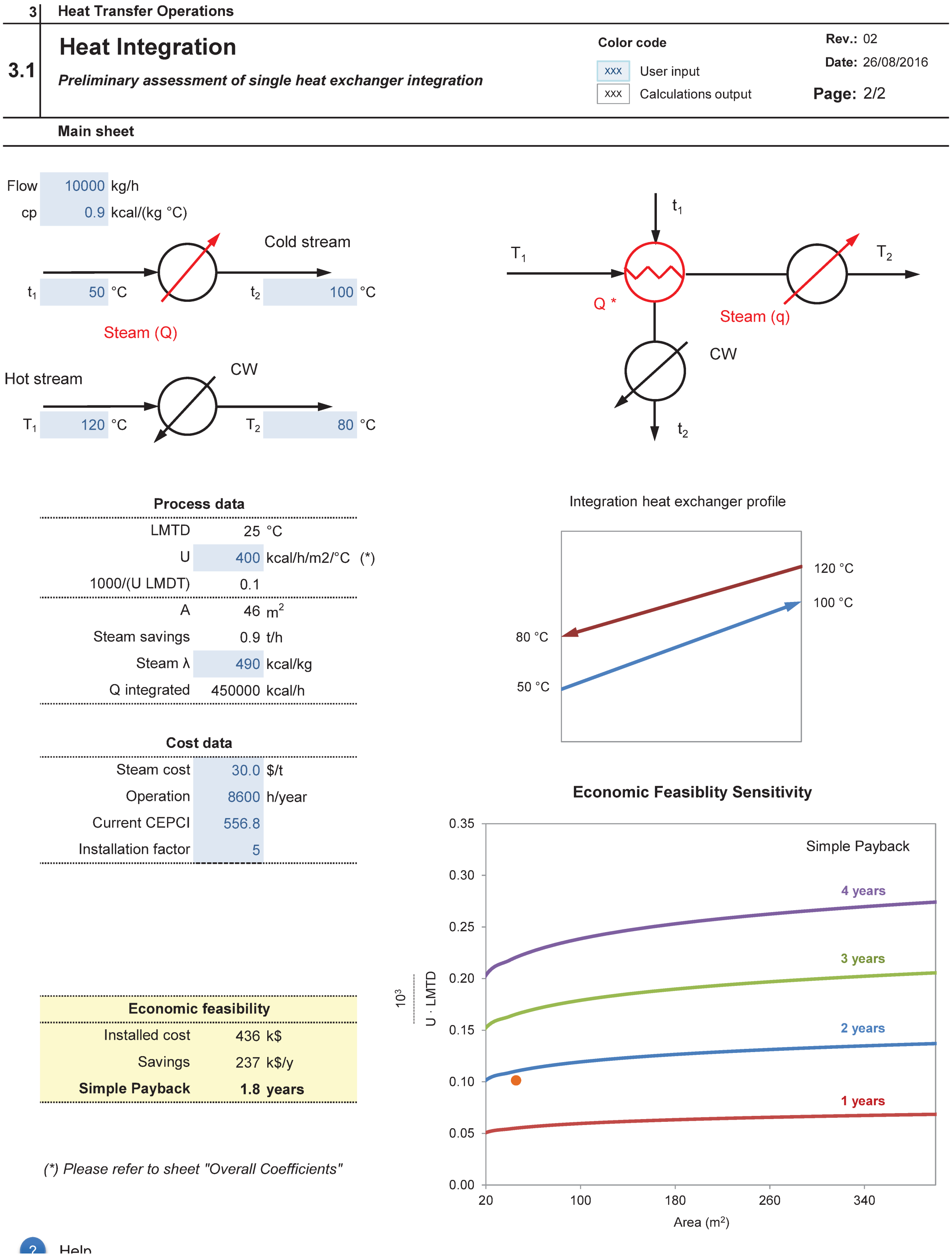
Cost data		
Installation Factor	3	
Current CEPCI	556.8	
Steam cost	30.0	$/t
	14.6	$/GJ
Electricity cost	0.15	$/kWh
	41.7	$/GJ
$ Power / $ Steam	2.8	

Performance data		
ΔT_{appro}	30	°C
ΔT_{column}	45	°C
T_{out}	172	°C
P_{out}	7.1	bar a
COP_{max}	5.4	
η_{over}	75%	
COP	4.1	
Required heat	980	Mcal/h
Available heat	750	Mcal/h
Power required	281	kW

Economic Feasibility		
Installed cost	2055	k$
Operating Cost (Conventional)	516	k$/year
Operating Cost (VRC)	362	k$/year
Simple Payback	**13.4**	**years**

B.3 Heat transfer operations

B.3.1 Thermal Integration



3 **Heat Transfer Operations**

3.1 **Heat Integration**

Preliminary assessment of single heat exchanger integration

Color code	
xxx	User input
xxx	Calculations output

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Main sheet

Flow	10000	kg/h
cp	0.9	kcal/(kg °C)

Cold stream

t_1	50	°C
t_2	100	°C

Steam (Q)

Hot stream

CW

T_1	120	°C
T_2	80	°C

Process data

LMTD	25	°C
U	400	kcal/h/m2/°C (*)
1000/(U LMDT)	0.1	
A	46	m^2
Steam savings	0.9	t/h
Steam λ	490	kcal/kg
Q integrated	450000	kcal/h

Cost data

Steam cost	30.0	$/t
Operation	8600	h/year
Current CEPCI	556.8	
Installation factor	5	

Economic feasibility

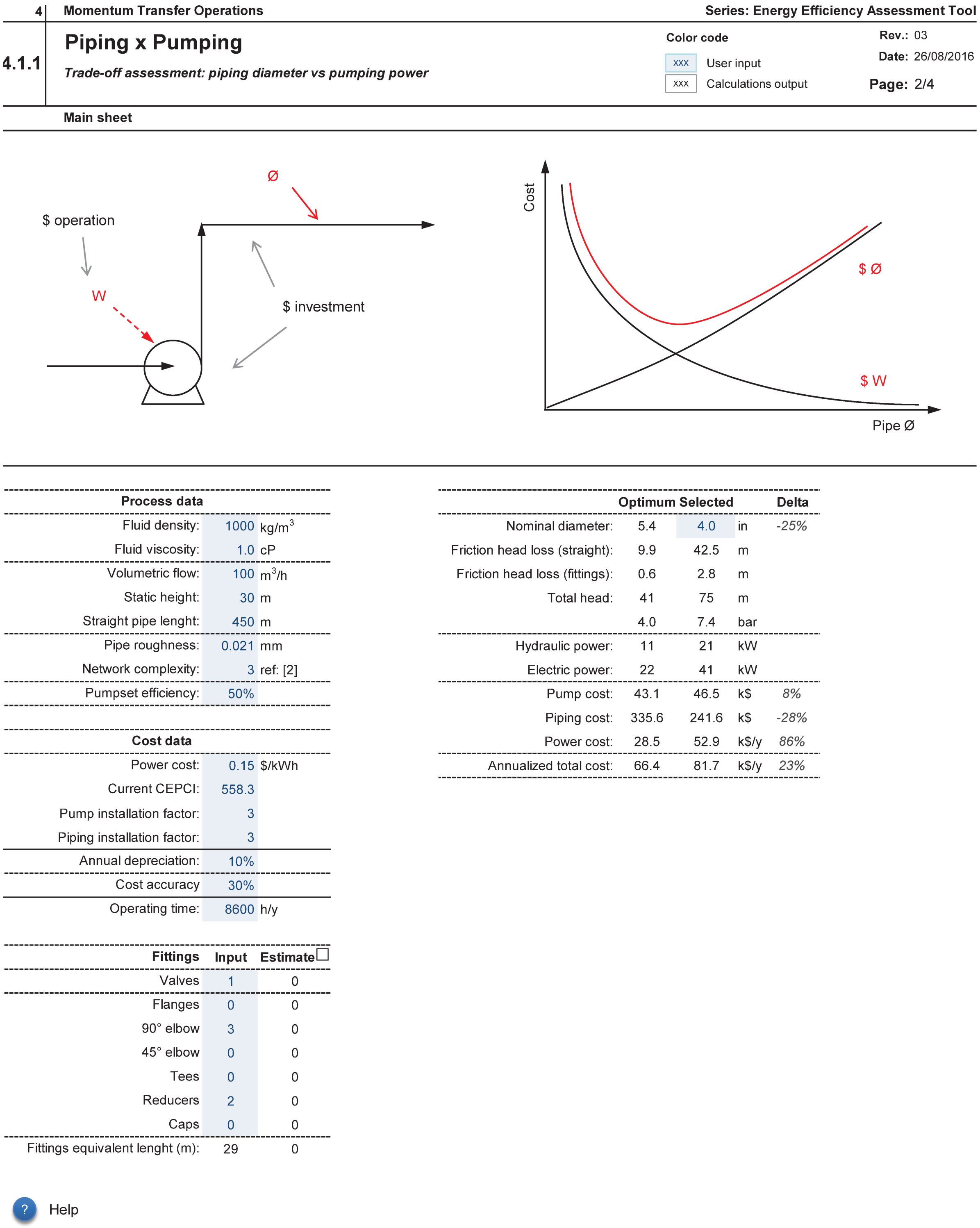
Installed cost	436	k$
Savings	237	k$/y
Simple Payback	**1.8**	**years**

(*) Please refer to sheet "Overall Coefficients"

? Help

B.4 Momentum transfer operations

B.4.1 Pumping systems



4 **Momentum Transfer Operations**

Series: Energy Efficiency Assessment Tool

4.1.1

Piping x Pumping

Trade-off assessment: piping diameter vs pumping power

Color code

xxx User input

xxx Calculations output

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Main sheet

Process data		
Fluid density:	1000	kg/m^3
Fluid viscosity:	1.0	cP
Volumetric flow:	100	m^3/h
Static height:	30	m
Straight pipe lenght:	450	m
Pipe roughness:	0.021	mm
Network complexity:	3	ref: [2]
Pumpset efficiency:	50%	

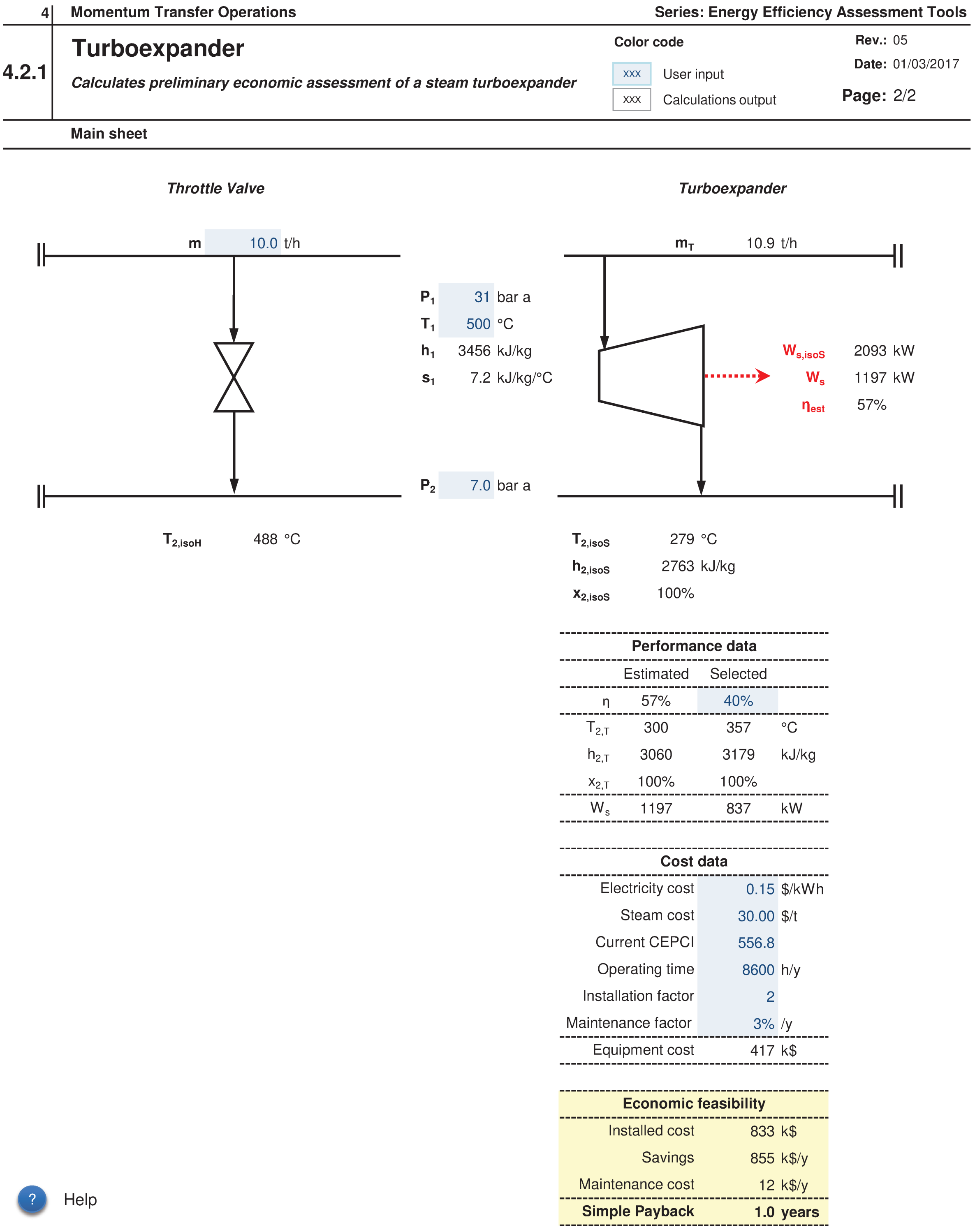
Cost data		
Power cost:	0.15	$/kWh
Current CEPCI:	558.3	
Pump installation factor:	3	
Piping installation factor:	3	
Annual depreciation:	10%	
Cost accuracy	30%	
Operating time:	8600	h/y

Fittings	Input	Estimate ☐
Valves	1	0
Flanges	0	0
90° elbow	3	0
45° elbow	0	0
Tees	0	0
Reducers	2	0
Caps	0	0
Fittings equivalent lenght (m):	29	0

	Optimum	Selected		Delta
Nominal diameter:	5.4	4.0	in	*-25%*
Friction head loss (straight):	9.9	42.5	m	
Friction head loss (fittings):	0.6	2.8	m	
Total head:	41	75	m	
	4.0	7.4	bar	
Hydraulic power:	11	21	kW	
Electric power:	22	41	kW	
Pump cost:	43.1	46.5	k$	*8%*
Piping cost:	335.6	241.6	k$	*-28%*
Power cost:	28.5	52.9	k$/y	*86%*
Annualized total cost:	66.4	81.7	k$/y	*23%*

Help

B.4.2 Steam turboexpansion



4 **Momentum Transfer Operations**

Series: Energy Efficiency Assessment Tools

4.2.1

Turboexpander

Calculates preliminary economic assessment of a steam turboexpander

Color code

xxx User input

xxx Calculations output

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Main sheet

Throttle Valve

Turboexpander

m 10.0 t/h

$\mathbf{m_T}$ 10.9 t/h

$\mathbf{P_1}$ 31 bar a

$\mathbf{T_1}$ 500 °C

$\mathbf{h_1}$ 3456 kJ/kg

$\mathbf{s_1}$ 7.2 kJ/kg/°C

$W_{s,isoS}$ 2093 kW

W_s 1197 kW

η_{est} 57%

$\mathbf{P_2}$ 7.0 bar a

$\mathbf{T_{2,isoH}}$ 488 °C

$\mathbf{T_{2,isoS}}$ 279 °C

$\mathbf{h_{2,isoS}}$ 2763 kJ/kg

$\mathbf{x_{2,isoS}}$ 100%

Performance data

	Estimated	Selected	
η	57%	40%	
$T_{2,T}$	300	357	°C
$h_{2,T}$	3060	3179	kJ/kg
$x_{2,T}$	100%	100%	
W_s	1197	837	kW

Cost data

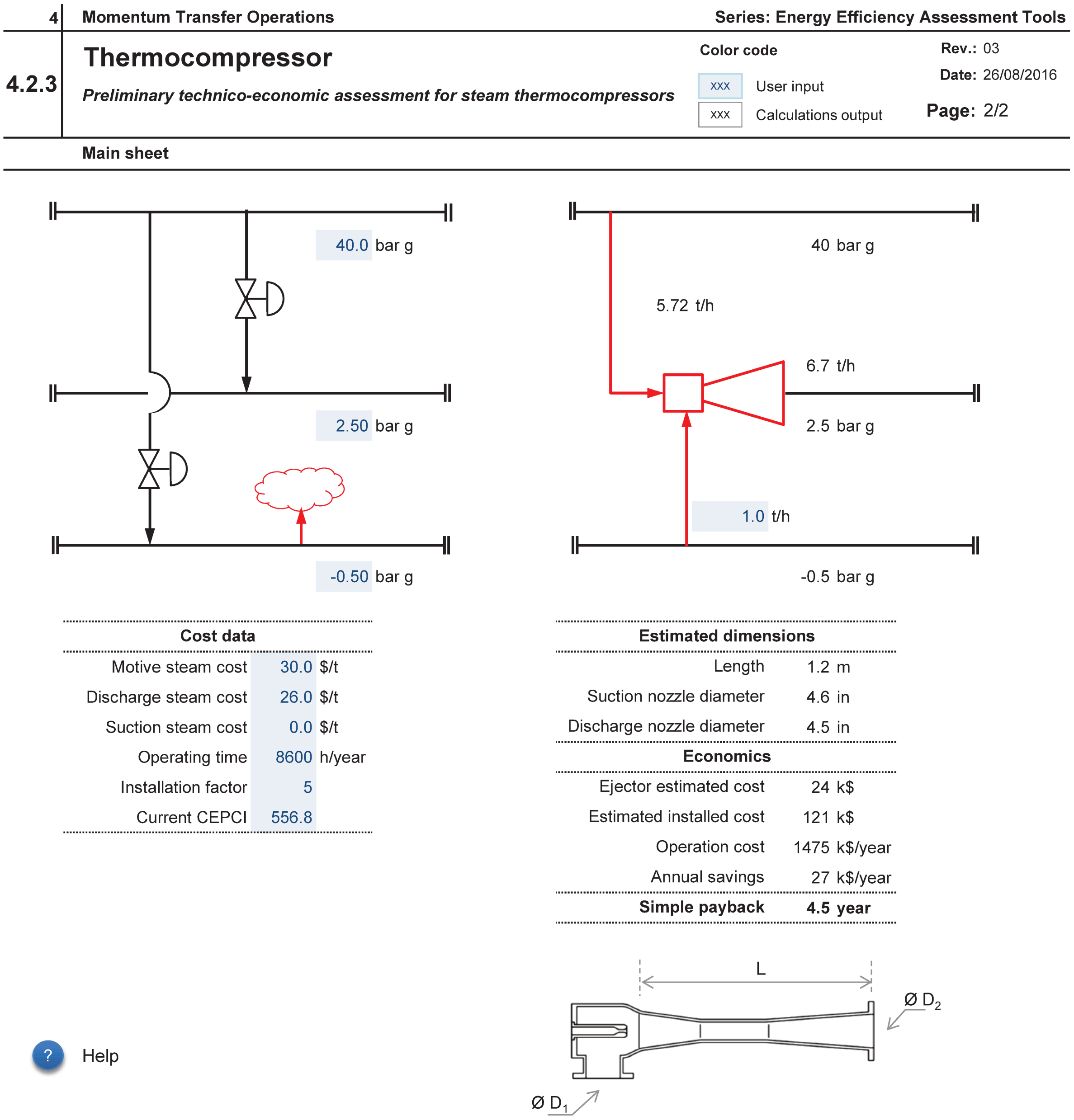
Electricity cost	0.15	$/kWh
Steam cost	30.00	$/t
Current CEPCI	556.8	
Operating time	8600	h/y
Installation factor	2	
Maintenance factor	3%	/y
Equipment cost	417	k$

Economic feasibility

Installed cost	833	k$
Savings	855	k$/y
Maintenance cost	12	k$/y
Simple Payback	**1.0**	**years**

? Help

B.4.3 Steam thermocompression



4 **Momentum Transfer Operations**

Series: Energy Efficiency Assessment Tools

4.2.3

Thermocompressor

Preliminary technico-economic assessment for steam thermocompressors

Color code

xxx User input
xxx Calculations output

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Main sheet

40.0 bar g
2.50 bar g
-0.50 bar g

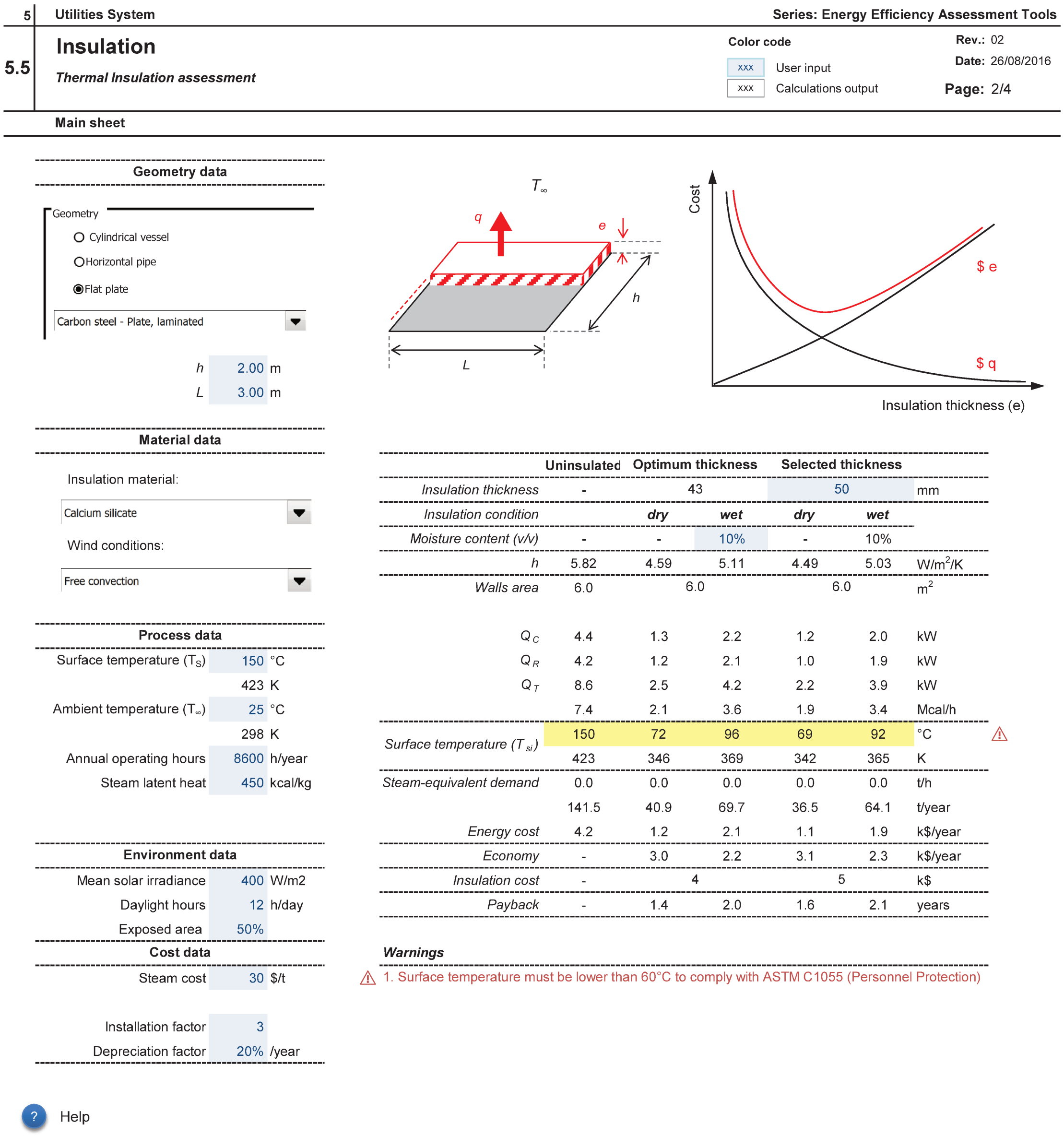
40 bar g
5.72 t/h
6.7 t/h
2.5 bar g
1.0 t/h
-0.5 bar g

Cost data		
Motive steam cost	30.0	$/t
Discharge steam cost	26.0	$/t
Suction steam cost	0.0	$/t
Operating time	8600	h/year
Installation factor	5	
Current CEPCI	556.8	

Estimated dimensions		
Length	1.2	m
Suction nozzle diameter	4.6	in
Discharge nozzle diameter	4.5	in
Economics		
Ejector estimated cost	24	k$
Estimated installed cost	121	k$
Operation cost	1475	k$/year
Annual savings	27	k$/year
Simple payback	**4.5**	**year**

B.5 Utilities systems

B.5.1 Thermal insulation



5 **Utilities System** **Series: Energy Efficiency Assessment Tools**

5.5 **Insulation**

Thermal Insulation assessment

Color code

xxx User input
xxx Calculations output

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Main sheet

Geometry data

Geometry
○ Cylindrical vessel
○ Horizontal pipe
● Flat plate

Carbon steel - Plate, laminated

h	2.00	m
L	3.00	m

Material data

Insulation material:

Calcium silicate

Wind conditions:

Free convection

Process data

Surface temperature (T_S)	150	°C
	423	K
Ambient temperature (T_∞)	25	°C
	298	K
Annual operating hours	8600	h/year
Steam latent heat	450	kcal/kg

Environment data

Mean solar irradiance	400	W/m2
Daylight hours	12	h/day
Exposed area	50%	

Cost data

Steam cost	30	$/t
Installation factor	3	
Depreciation factor	20%	/year

	Uninsulated	**Optimum thickness**		**Selected thickness**		
Insulation thickness	-	43		50		mm
Insulation condition		***dry***	***wet***	***dry***	***wet***	
Moisture content (v/v)	-	-	10%	-	10%	
h	5.82	4.59	5.11	4.49	5.03	$W/m^2/K$
Walls area	6.0	6.0		6.0		m^2
Q_C	4.4	1.3	2.2	1.2	2.0	kW
Q_R	4.2	1.2	2.1	1.0	1.9	kW
Q_T	8.6	2.5	4.2	2.2	3.9	kW
	7.4	2.1	3.6	1.9	3.4	Mcal/h
Surface temperature (T_{si})	150	72	96	69	92	°C ⚠
	423	346	369	342	365	K
Steam-equivalent demand	0.0	0.0	0.0	0.0	0.0	t/h
	141.5	40.9	69.7	36.5	64.1	t/year
Energy cost	4.2	1.2	2.1	1.1	1.9	k$/year
Economy	-	3.0	2.2	3.1	2.3	k$/year
Insulation cost	-	4		5		k$
Payback	-	1.4	2.0	1.6	2.1	years

Warnings

⚠ 1. Surface temperature must be lower than 60°C to comply with ASTM C1055 (Personnel Protection)

Appendix C

Cost curves

Heat pump assisted distillation

$$C_{\text{compressor}} = 46308 \cdot W^{0.82} \text{ [US\$ @ 1986 - From MESZAROS and FONYO (1986)]}$$

$$C_{\text{exchanger}} = 2790 \cdot A^{0.65} \text{ [US\$ @ 1986 - From MESZAROS and FONYO (1986)]}$$

Thermal Integration

$$C_{\text{exchanger}} = 2000 \cdot A^{0.9} \text{ [US\$ @ 2012 - From COUPER (2012)]}$$

Pumping systems

$$C_{\text{pump}} = 1.39 \cdot \exp\left(8.833 - 0.6019 \cdot \ln(Q \cdot H^{0.5}\right) + 0.0519 \cdot \ln(Q \cdot H^{0.5})^2)$$

[US$ @ 2003 - From COUPER (2012)]

$C_{\text{piping}} = (0.0987{\cdot}D^2{+}4.1159{\cdot}D{-}0.39)/550.8$ [US$ / 100m @ 2014 - From internal data]

Steam turboexpansion

$$C_{\text{turbine}} = 3462.7 \cdot W^{0.7145} \text{ [US\$ @ 2013 - From COUPER (2012)]}$$

Steam thermocompression

$$C_{\text{ejector}} = 10000 + 600 \cdot D^{1.2} \text{ [US\$ @ 1992 - Adapted from POWER (1994)]}$$

$$D = 0.26 \cdot \max((WD/PD)^{0.5}, (WS/PS)^{0.5})$$

where W are in lb/h and P in psia

Thermal insulation

$$C_{\text{Calcium Silicate}} = \$15\,/\mathrm{m}^2 \text{ [US\$ @ 2014 - From internal data]}$$

$$C_{\text{PU}} = \$2000\,/\mathrm{m}^3 \text{ [US\$ @ 2014 - From internal data]}$$