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Towards the Use of Mathematical Optimization for Work and Heat Exchange Networks

Matias Vikse[a,*], Chao Fu[b], Paul I. Barton[c], Truls Gundersen[a]

[a]Norwegian University of Science and Technology, Department of Energy and Process Engineering, Kolbjoern Hejes vei 1A, NO-7491 Trondheim, Norway
[b]SINTEF Energy Research, Kolbjoern Hejes vei 1A, NO-7491 Trondheim, Norway
[c]Massachusetts Institute of Technology, Process Systems Engineering Laboratory, Cambridge, MA 02139
matias.vikse@ntnu.no

Pinch Analysis is a well-known methodology that has achieved great success in increasing process efficiency since its inception in the 1970s. The traditional approach in Pinch Analysis has mainly been concerned with Heat Integration. However, most chemical processes also consist of pressure-changing units such as compressors, expanders and valves, which will influence the Heat Integration in the process. The problem is extended to that of Work and Heat Integration, a research topic that has gained a lot of interest recently. Pressure manipulation of streams affects the stream temperatures and thus the Heat Integration problem. Furthermore, the inlet temperature to expanders and compressors determines the power produced or consumed. The Work and Heat Integration problem is thus much more complex than Heat Integration alone, and a manual procedure is only possible for very small problems. To handle larger industrial problems and to properly handle the complex trade-offs involved, rigorous optimization models are necessary. This paper studies three existing superstructures for modeling Work and Heat Exchange Networks. It also looks at possible Pinch location algorithms that can be included in the models. Finally, the paper presents the disadvantages in each of the three modeling approaches, indicating the need for a new superstructure.

1. Introduction

Pinch Analysis is a well-known methodology in Process Integration for designing Heat Exchanger Networks (HENs) since its inception in the 1970s. The methodology has been successfully applied both to novel process designs as well as retrofitting with significant improvements in energy efficiency. Aiding the calculations, mathematical programming has frequently been used, where Pinch location algorithms have been developed, such as the transshipment model (Papoulias and Grossmann, 1983) and the simultaneous optimization and heat integration approach for chemical processes (Duran and Grossmann, 1986).
Despite its apparent success in the industry, Pinch Analysis has a disadvantage in that it only considers Heat Integration and neglects the effect of pressure manipulations. As most chemical processes contain pressure-changing units such as compressors, expanders, valves, etc., it is important to also consider how these units influence the HEN. The concept of Appropriate Placement (Townsend and Linnhoff, 1983), commonly referred to as Correct Integration, is a fundamental principle in Pinch Analysis. Enhanced heat recovery can be obtained by integrating various process equipment types in the HEN. However, if done incorrectly it could have a negative effect on the efficiency. The Appropriate Placement of various equipment such as heat engines, heat pumps, reactors and distillation columns in HENs is already well documented (Smith, 2016). The integration of compressors and expanders is more complex, however, as it involves both work and heat transfer. The ExPAnD methodology (Aspelund et al., 2007) addressed this issue by introducing the heuristic rule that compression adds heat to the system and should be done above Pinch, while expansion adds cooling and should be done below Pinch. Later, Gundersen et al. (2009) formulated this more precisely by saying that compression and expansion should start at the Pinch. This heuristic was embedded in the superstructure used for optimization of Work and Heat Exchange Networks (Wechsung et al., 2011). In order to correctly quantify the contributions from thermal utilities (heat) and the pressure manipulating equipment (work), exergy rather than energy was used for

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targeting in these models. The heuristic rule has a limited validity, however, and can result in suboptimal solutions if used without care. Therefore, a set of theorems was developed for Appropriate Placement of compressors (Fu and Gundersen, 2015a) and expanders (Fu and Gundersen, 2015b) in above ambient processes and for compressors (Fu and Gundersen, 2015c) and expanders (Fu and Gundersen, 2015d) in sub-ambient processes. The theorems concluded that compression/expansion should start at Pinch, ambient, or cold/hot utility temperatures depending on the design problem. Several test examples were used to illustrate these theorems using a manual design procedure and the Grand Composite Curve (GCC). However, as the GCC changes when including the pressure-manipulated streams, a graphical approach is only possible for small problems. Thus, a rigorous optimization model is necessary for studying larger problems, where a sufficiently rich superstructure includes the alternative network configurations.

2. Superstructures used for optimization of Work and Heat Exchange Networks

Wechsung et al. (2011) use a state space approach to modeling WHENs, in which the HEN and the pressure-changing equipment are separated into different operations. There is a Pinch operator that locates the Pinch point(s) and calculates the minimum utility requirements for the process streams. The Pinch operator also prevents violation of the minimum temperature difference in the heat exchangers. Compression and expansion are included through the pressure operator. The objective of the model is to minimize exergy consumption.
The process streams in the model are either fixed or variable (see Figure 1). The fixed streams are streams that do not undergo any pressure change, and thus only interact with the Pinch operator. The variable streams, on the other hand, are the set of streams that undergo pressure change, and will therefore interact with both Pinch and pressure operators. Wechsung et al. (2011) employed the ExPAnD methodology in the development of a compression/expansion scheme. Their focus was on sub-ambient processes, particularly for Liquefied Natural Gas (LNG), where cooling is the primary objective. The proposed superstructure has a compression/expansion scheme (with three stages) for hot streams: cooling, compression, cooling, expansion, heating, compression and then cooling to target temperature. Similarly, for cold streams and the same number of stages: heating, expansion, heating, compression, cooling, expansion and heating to target temperature. Stream segments are used for each of the different pressure-stages in the model, with variable supply and target temperatures. Hence, the model requires a Pinch location algorithm that is capable of handling variable supply/target temperatures (see Section 3). The compression/expansion scheme causes stream identity changes to occur in the model. For instance, the variable hot stream is temporarily a cold stream after expander EX1, before changing back to being a hot stream after compressor CO2. Similarly, the variable cold stream turns into a hot stream after compressor CO3 before returning to be a cold stream after expander EX3.

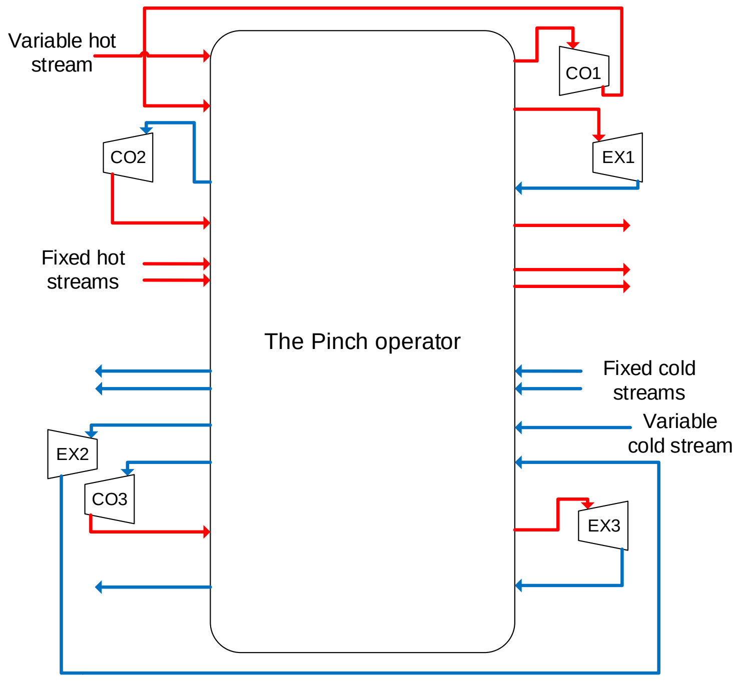

Figure 1: The superstructure by Wechsung et al. (2011) for WHENs

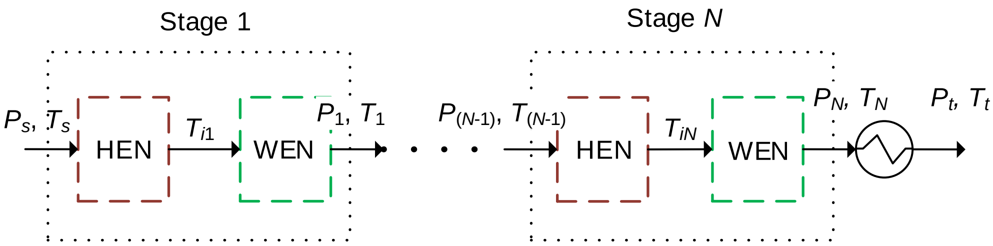

Figure 2: The multi-stage superstructure by Huang and Karimi (2016)

Huang and Karimi (2016) propose an alternative superstructure that, similarly to Wechsung et al. (2011), separates the problem into a HEN part and a compression/expansion part. Rather than reducing the exergy consumption, the objective of the model is to minimize Total Annual Cost of the process. The compression/expansion part is formulated as a Work Exchange Network (WEN) problem (Huang and Fan, 1996), allowing for pressure recovery from using companders (i.e. a unit with both expansion and compression). The result is the multi-stage superstructure shown in Figure 2, where the pressure-changing streams pass through the HEN and WEN at each pressure stage. P_s and T_s are the supply pressure and temperature, T_{in} is the intermediate temperature at stage n (where n = 1,…,N), and P_t and T_t are the target pressure and temperature. Rather than using the compression/expansion scheme of Wechsung et al. (2011), the model distinguishes between high-pressure (HP) and low-pressure (LP) streams. The HP streams are expanded, whereas the LP streams are compressed. The model also includes throttling valves for the HP streams as well as the possibility of bypassing pressure-changing stages (see Figure 3).

The model by Huang and Karimi (2016) does not employ the ExPAnD methodology for heat. Instead, the authors recognize that power production in expanders increases with increasing inlet temperature, whereas power consumption in compressors decrease with decreasing temperature. HP and LP streams are thus treated respectively as cold and hot streams in the HEN. Like the superstructure by Wechsung et al. (2011), this model requires a Pinch location algorithm to handle variable supply and target temperatures (Section 3).

A third superstructure for WHENs was developed by Maurstad Uv (2016) that incorporates the results of the theorems by Fu and Gundersen (2015a-d). The model only considers the integration of a single compressor/expander, and splits each pressure-changing stream into N branches, each consisting of two segments; one before and one after the pressure-changing unit (see Figure 4). The first segment will have a supply temperature equal to the supply temperature of the original stream and a target temperature corresponding to the inlet temperature of the pressure-changing unit, which is determined by the theorems. Consequently, a branch is needed for every Pinch temperature (located using the heat cascade), hot or cold utility temperature, and the ambient temperature. Similarly, supply and target temperatures of the second segment are equal to the outlet temperature of the pressure-changing unit and the target temperature of the original stream, respectively.

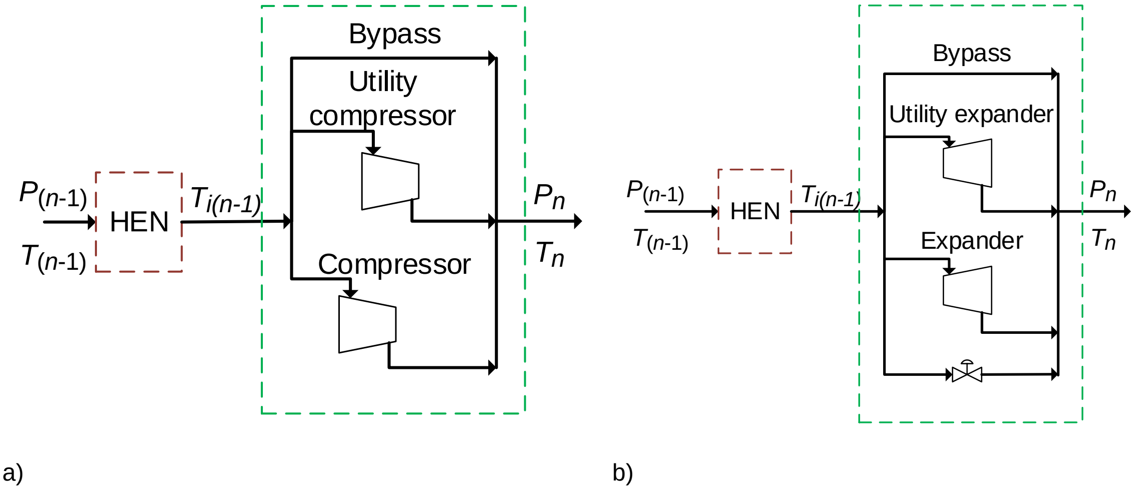

Figure 3: The WEN network at pressure stage n in the model by Huang and Karimi (2016): a) for low-pressure streams, b) for high-pressure streams

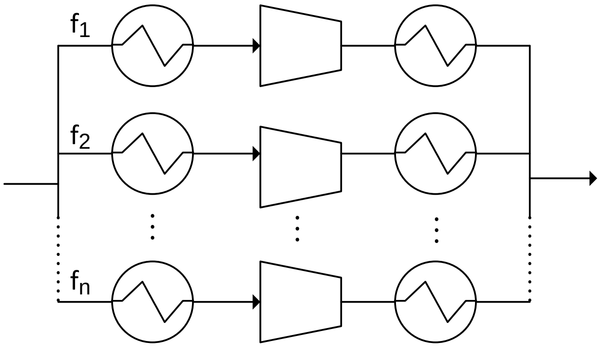

Figure 4: The superstructure by Maurstad Uv (2016)

3. Pinch operators

As mentioned in Section 2, the models by Wechsung et al. (2011) and later Huang and Karimi (2016) require a Pinch operator capable of handling variable supply and target temperatures. Several such algorithms exist, among them the models by Yee and Grossmann (1990) and Grossmann et al. (1998). Wechsung et al. (2011) used the latter as a Pinch operator in their model. It is a Mixed Integer Nonlinear Programming (MINLP) model with logic disjunctions for modeling the location of streams relative to potential Pinch Points. The big M formulation is used in the modeling of the disjunctive constraints, which can make the models hard to solve due to large relaxation gaps.
Onishi et al. (2014) developed an alternative model based on the same superstructure, but with the Pinch model by Yee and Grossmann (1990). This Pinch location method potentially matches each hot stream with every cold stream in a pre-defined number of stages. The result is an MINLP model with binary variables used for modeling possible heat exchange. Consequently, it solves for the HEN synthesis problem, the Pinch location problem, and obtains the total heat exchanger area simultaneously, and is thus suitable for optimization with respect to Total Annual Cost. These additional features come with increased complexity, however, and the model by Yee and Grossmann (1990) is comparatively more difficult to solve.
The simultaneous optimization and heat integration model by Duran and Grossmann (1986) is among the most notable in Process Integration. The model is a nonlinear program (NLP) that uses non-smooth equations instead of disjunctive constraints for identifying the placement of streams relative to a Pinch candidate. The result is a much smaller model than the MINLP formulations presented above. However, the difficulty lies in the non-smooth equations, which are non-differentiable at certain points. One possibility is to use smooth approximations, although the choice of parameters in the approximations can often be non-trivial and affect the solvability of the model (Grossmann et al., 1998). Alternatively, non-smooth optimization algorithms, e.g. bundle methods (Mäkelä and Neittaanmäki, 1992) have been developed that use generalized derivatives in place of conventional derivatives. Generalized derivatives are extensions of the concept of derivatives to some classes of non-differentiable functions, e.g. piecewise continuously differentiable functions, which include the non-smooth max and min operators used in the model by Duran and Grossmann (1986). Khan and Barton (2015) developed a method for calculating such generalized derivatives for piecewise continuously differentiable functions that is analogous to the vector forward mode in automatic differentiation. Watson et al. (2015) reformulated the model by Duran and Grossmann for implementation in a non-smooth multi-stream heat exchanger model. The alternative formulation removes the inequality constraints for the Pinch candidates in the original model and thus obtains a much better scaling.

4. Limitations of the superstructures

Wechsung et al. (2011) utilize the ExPAnD methodology in the superstructure where compression and expansion are integrated at the Pinch. According to the previously mentioned theorems, however, Pinch compression/expansion is not always optimal. Instead, stream splitting is sometimes required with inlet temperature to the pressure-changing unit being Pinch temperatures, hot or cold utility temperatures or ambient temperature. Therefore, not accounting for stream splitting in the superstructure may lead to suboptimal results.
Two recent approaches have included stream splitting in their superstructures. A model by Huang and Karimi (2016) splits streams to account for utility compressors or expanders, single shaft compressor-expander arrangements, a bypass, plus an additional branch for valves in the case of HP streams. The optimal integration of the WEN determines the stream split ratios in the network. Nevertheless, the inlet temperatures to the various pressure-changing units remain equal between the branches and thus the superstructure does not follow the

theorems for Correct Integration by Fu and Gundersen (2015a-d). Instead, the model maximizes power production in expanders by increasing the inlet temperature before expansion, and minimizes the power consumption in compressors by reducing the temperature before compression. Consequently, the superstructure considers the WEN and HEN parts separately, which may lead to suboptimal solutions at least in terms of total exergy consumption. Another difficulty with this formulation is the coupling of compressors and expanders. Additional binary variables are required to accommodate this additional feature, and thus the MINLP can become difficult to solve for large problems. Binary variables are also included for generators, helper motors, utility compressors/expanders, valves, and bypasses on each stage, thus adding further complexity to the model. Although these extra features are required when minimizing Total Annual Cost, they add unnecessary complexity to exergy targeting models.

In the superstructure by Maurstad Uv (2016), each stream branch corresponds to a possible inlet temperature to the pressure-changing unit, i.e. a Pinch Temperature, hot or cold utility temperature or ambient temperature. The Pinch Points are calculated from the heat cascade prior to optimization. The algorithm by Maurstad Uv (2016) is sequential, following the same calculation procedure as Fu and Gundersen (2015 a-d). The result was a linear model that is easy to solve. However, this sequential solution strategy has several disadvantages. Integrating more than one compressor/expander sequentially can potentially lead to suboptimal results as the integration sequence might influence the set of Pinch Points in the network. Each possible sequence of integration should be studied in order to ensure global optimality, which can be tedious. Another problem occurs whenever the heat from compression or the cooling from expansion exceeds the heat deficit or surplus at the given temperature in the process. In this case, a new Pinch point occurs, and more stream branches are required. Several additional Pinch Points may occur with pressure integration, in which case the heat cascade must be solved multiple times before reaching an appropriate number of stream splits in the model. Alternatively, a state space approach similar to the models by Wechsung et al. (2011) and Huang and Karimi (2016) can be employed. In that case, a sequential approach is no longer necessary. The penalty is that a nonconvex NLP model (in case of non-smooth Pinch location algorithms) or an MINLP model will replace the much simpler LP model. In addition, the proposed superstructure with stream branches for every Pinch point in the model will be problematic in the simultaneous approach. Pinch Points may be created or changed due to the integration of pressure-manipulated streams in the model. The number of branches, and thus stream segments, may also change during optimization. This further complicates the problem, as the final number of variable hot or cold streams (segments) is unknown.

5. Conclusions

This paper studies three alternative optimization models for Work and Heat Exchange Networks. The first two models by Wechsung et al. (2011) and Huang and Karimi (2016) use a state space approach in which the WHEN problem is divided into different operations (pressure manipulation and heat integration). The third model by Maurstad Uv (2016) is based on a sequential approach, using the heat cascade for locating Pinch points.

Any simultaneous optimization and heat integration algorithm can be employed as a Pinch operator, though it may affect the efficiency of the model. Possible Pinch operators are the non-smooth NLP models by Duran and Grossmann (1986), or the reformulation by Watson et al. (2015) and the MINLP models by Yee and Grossmann (1990) and Grossmann et al. (1998). Of the MINLP models, the last formulation contains fewer binary variables and is easier to solve. The MINLP models obtain a worse scaling than the non-smooth Pinch location methods by Duran and Grossmann (1986) and much later Watson et al. (2015). These models, however, consist of equations that are not differentiable everywhere. Smooth approximations have frequently been used to deal with non-differentiabilities. However, the choice of parameters for the smoothing function can be non-trivial, and may affect the solvability of the model. Recent developments in non-smooth analysis have focused on calculating generalized derivatives for these types of functions. Generalized derivatives may be used in place of conventional derivatives in bundle solvers for non-smooth optimization, avoiding the numerical difficulties from using smooth approximations.

The models by Wechsung et al. (2011) and Huang and Karimi (2016) do not consider the theorems for Correct Integration of pressure-changing equipment, and suboptimal results may thus be obtained. This issue is addressed in the third superstructure by Maurstad Uv (2016). Although the resulting model was an LP, which is easy to solve, its sequential approach has several drawbacks. In particular, pressure manipulations may create additional Pinch Points, requiring several iterations of the pre-processing procedure. Furthermore, the sequence of integration may also influence the set of Pinch locations and thus the solution of the model. On the other hand, a simultaneous approach is also difficult with this superstructure, primarily due to the fact that the number of stream branches and stream segments changes in the model. Further research is therefore required to establish a superstructure that (1) builds on the theorems for Correct Integration, (2) works well with a simultaneous approach, and (3) scales well with the number of streams and pressure-changing equipment such that the model can be applied to larger and more commercially interesting process designs.

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