A Nonsmooth Formulation for Handling Unclassified Process Streams in the Optimization of Work and Heat Exchange Networks (WHENs)

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Abstract

Pinch Analysis provides a systematic methodology for improving efficiency through enhanced process integration. Originally, the methodology focused on heat integration with Heat Exchanger Network (HEN) synthesis. However, most chemical processes also include pressure manipulation with the inclusion of equipment such as compressors, expanders, pumps and valves that affect heat integration. Recently, attention has therefore been directed towards simultaneous work and heat integration and the synthesis of Work and Heat Exchange Networks (WHENs). Mathematical Programming has proven effective in solving heat integration problems. Several pinch location algorithms exist in the literature that calculate the minimum utility consumption given a set of hot and cold process streams. However, classification of streams into hot and cold streams prior to optimization is difficult when integrating compressors and expanders in HENs. Depending on the integration problem, the compression/expansion temperatures can vary greatly in order to fully utilize the heat of compression (or cooling from expansion) in the process. This represents a modeling issue, as classifying the stream identities prior to optimization essentially impose an upper or lower bound on the temperature variable. Instead, pinch location algorithms must be modified to handle unclassified process streams. Different strategies for handling unclassified process streams in exergy targeting and synthesis of WHENs were proposed by Yu *et al.* This article presents an alternative and more compact formulation using a nonsmooth extension to the simultaneous optimization and heat integration algorithm by Duran and Grossmann in order to handle unclassified process streams. Optimization is performed using IPOPT and the sensitivities (gradients) are obtained using recent developments in nonsmooth analysis. The nonsmooth extension is tested for WHEN targeting using a number of examples from the literature.

Introduction

Pinch Analysis is well-known in process integration for designing Heat Exchanger Networks (HENs) since its inception in the 1970s, and has been applied both to novel process designs as well as retrofitting with significant success in improving the energy efficiency. The point with the smallest temperature difference ΔT_{min} between the hot and cold composite curves is known as the pinch point for the process. Furthermore, at minimum utility consumption, the composite curves are decomposed at the pinch point, where the region above pinch has a net heat deficit, whereas the region below pinch has a net heat surplus. Consequently, any heat transfer across the pinch point will require additional hot and cold utilities, and should be prevented for minimum energy targeting. The success of Pinch Analysis and heat integration has attracted a continued interest in further improving the methodology. Extensive reviews on HEN synthesis have been presented by Gundersen and Naess,[1] Furman and Sahinidis,[2] and more recently by Klemeš and Kravanja.[3]

Although Pinch Analysis has resulted in significant improvements in energy efficiency of industrial processes, it suffers from significant limitations in that it only considers heat integration. However, most chemical processes contain pressure-changing equipment such as compressors, expanders, pumps and valves that influence the heat integration problem. Huang and Fan[4] extended the concept of heat exchanger networks to that of work exchange networks (WENs), where work is transferred from high pressure to low pressure streams using flow work exchangers. Later, Razib *et al.*[5] developed a model for WEN synthesis, where compressors and expanders are matched using single shaft turbine compressors (SSTCs). The model also included utility compressors and expanders, as well as valves. Heat integration is not considered in their WEN synthesis problem. However, pressure-changing equipment also change the temperatures of the streams and thus affect the scope for heat recovery. Therefore, rather than looking at heat integration and work integration separately, they should be optimized simultaneously, in what is known as a Work and Heat Exchange Networks (WHENs).

Appropriate placement,[6] also commonly referred to as correct integration, is an important concept in Pinch Analysis. Enhanced heat recovery can be obtained by integrating various process equipment types in the HEN. However, integrating process equipment incorrectly could lower the overall thermal efficiency. Consequently, explicit rules for the integration of different process units must be documented to take full advantage of the benefits of process integration. Rules for integrating heat engines, heat pumps, reactors and distillation columns in HENs are already well documented.[7] Along with the increased interest in simultaneous work and heat integration, rules for appropriate placement of compressors and expanders have been studied in detail. Pressure-changing equipment change stream temperatures as well as pressures, and thus the shape of the composite curves. As a result, the integration of compressors and expanders is considerably more complex than other process equipment, where only the operating temperatures are of concern. Heuristic rules for the integration of compressors and expanders were included in the ExPAnD methodology.[8] As compression adds heat to the system and expansion provides cooling, the authors concluded that compression should be done above pinch where there is a heat deficit, and expansion should preferably be done below pinch where there is a heat surplus. Later, the heuristics were formulated more precisely, saying that both compression and expansion should start at the pinch.[9] Fu and Gundersen developed a series of theorems for the appropriate placement of compressors[10] and expanders[11] in above ambient networks. Analogous theorems for the correct integration of compressors[12] and expanders[13] were also developed for subambient processes. Exergy analysis was used for proving the theorems. The theorems provide specific guidelines for the integration of compressors and expanders to minimize the total exergy destruction in the network. It was shown that pinch compression/expansion, as suggested by the ExPaND methodology, yield optimal results only for specific instances. In particular, the correct integration of pressure changing equipment depends on the heat (cooling) available at the compressor (expander) outlet temperature, as determined by the process' Grand Composite Curve. The theorems identify the possible inlet temperature candidates for the compressors/expanders. Depending on the problem, inlet temperatures for compression and expansion must be a combination of the pinch temperature(s), hot or cold utility temperature and ambient temperature. Therefore, stream splitting and compression/expansion at different temperatures is sometimes required for minimizing the exergy destruction in the network.

In addition, the authors developed a manual exergy targeting and design procedure for WHENs using the Grand Composite Curve as a design tool. The manual design procedure uses the guidelines provided by the theorems to develop a work and heat exchange network for which exergy destruction is minimized. Although the methodology is rigorous and guaranteed to obtain a global solution, its iterative nature makes it hard to use even for smaller problems. Specifically, each compressor/expander must be included successively, following a new heat cascade and Grand Composite Curve. As more variable pressure streams or stream splits are added to the problem, the heat cascades and Grand Composite Curves are expanded at every iteration, to the point of becoming limiting even for small scale problems. The development of a superstructure and mathematical optimization model, which include the thermodynamic insights from the theorems, is therefore necessary to efficiently perform exergy targeting and synthesis of WHENs.

Several optimization models for WHEN synthesis have been presented in the literature. Wechsung *et al.*[14] developed a superstructure for optimization of WHENs at subambient conditions. The superstructure assigns the pressure manipulations and heat integration to a pressure operator and pinch operator, respectively. Furthermore, an elaborate compression and expansion route is included, which is based on the heuristics provided by the ExPAnD methodology. The resulting model is a mixed integer nonlinear program (MINLP) for minimum exergy targeting of subambient processes. The same model was used for developing a process for offshore production of liquefied natural gas (LNG). Later, Onishi *et al.*[15] included the same superstructure for a Total Annualized Cost (TAC) analysis. The model was later extended to also include retrofit analysis of WHENs at sub-ambient process conditions.[16] Another superstructure for TAC analysis of WHENs was developed by Huang and Karimi,[17] where a WHEN is developed by synthesizing the WEN and HEN simultaneously. The WEN superstructure is adapted from the work of Razib *et al.*[5] and includes multistage compression and expansion, SSTCs, utility compressors/expanders, valves and bypass of the pressure stage. Another superstructure for TAC analysis and WHEN synthesis was developed by Nair *et al.*[18] The superstructure is richer and more general than the model proposed by Huang and Karimi. Specifically, the model allows for phase transitions, and the use of phase-based property models for the process streams. In addition, classification of streams into hot and cold streams, as well as high and low pressure streams is no longer required.[18]

In WHEN synthesis, compression and expansion temperatures are varying considerably, making it difficult to classify the variable pressure streams into hot and cold streams for heat integration. Simultaneous optimization and heat integration algorithms exist in the literature that handle unknown supply and target temperatures as part of the optimization problem. However, these algorithms normally regard the stream identities as known a priori. Different extensions for also handling cases where stream identities are unknown have been proposed. Yu *et al.*[19] tested different extensions to the simultaneous optimization and heat integration algorithm by Duran and Grossmann.[20] The authors presented three different modeling strategies. The first strategy used smooth approximations for the nonsmooth operators, and binary variables for the stream identities. The other two approaches replaced the nonsmooth operators with the disjunctive formulations by Grossmann *et al.*[21] and Quirante *et al.*[22] The authors concluded that the approach using smooth approximations performed better overall than the two disjunctive representations. Quirante *et al.*[23] presented an extension to the disjunctive pinch location algorithm[22] that handles unclassified streams, where disjunctions are included to assign the stream identity. The same formulation was later used by Onishi *et al.*[24] in an optimization model for WHEN synthesis with unclassified process streams. Nair *et al.*[18] allowed for unclassified process streams in the superstructure using a big-M formulation and solving an MINLP.

The present paper presents a nonsmooth extension to the Duran and Grossmann model for handling unclassified process streams. The nonsmooth operators max and min are used for assigning target temperatures for the variable temperature streams, and removing the contribution from streams with wrong identity. The main contribution of this work is that no binary variables or disjunctive formulations are required, resulting in a more compact formulation of the WHEN targeting and synthesis problem than the different formulations proposed by Yu *et al.*[19] The extension can be used both for the original Duran and Grossmann model and the reformulation by Watson *et al.*[25] Nonsmooth operators have normally been avoided in process modeling due to points of nondifferentiability, where the Jacobian is undefined. Nondifferentiable points represents an issue in derivative based solvers. Consequently, alternative modeling approaches such as smooth approximations or using disjunctions have traditionally been used for representing the nonsmooth functions. New advances in nonsmooth analysis introduced an alternative approach where sensitivities (gradients) of the nonsmooth functions are computed using an automatic differentiation methodology for Lexicographic Directional (LD-)derivatives.[26] The new nonsmooth extension is used for modeling different WHEN case studies presented in the papers by Fu and Gundersen.[10,11] Optimization is done using the primal-dual interior point algorithm IPOPT,[27] with sensitivities obtained analytically with the nonsmooth analog for automatic differentiation.[26]

Background

Superstructure for exergy targeting and WHEN synthesis

Yu *et al.* formulated the WHENs problem[28] as follows: "Given a set of process streams with supply and target states (temperature and pressure) as well as utilities for heating, cooling and power; design a Work and Heat Exchange Network consisting of heat transfer equipment such as heat exchangers, heaters and coolers, as well as pressure changing equipment such as compressors, expanders, pumps and valves, in a way that minimizes Exergy consumption or Total Annualized Cost". The interaction between pressure changing equipment and the heat exchanger network is therefore instrumental in analysing and designing WHENs. Pressure changes affect both temperature and pressure of the stream, and thus the possible heat integration in the network. Vice versa, the work input (or work output) from pressure changing equipment is dependent on the inlet temperature.

Theorems for appropriate placement of compressors[10] and expanders[11] were developed by Fu and Gundersen for above ambient networks. Similar theorems were also developed for integration of compressors[12] and expanders[13] in subambient processes. The theorems expanded on the heuristics provided by the ExPAnD methodology[8] and later in Gundersen *et al.*,[9] which stated that compression and expansion should always start at the process pinch point. However, Fu and Gundersen later discovered that pinch compression/expansion is not always optimal; one critical issue being whether the amount of heat or cooling can be absorbed by the process. Using exergy analysis, it was concluded that for minimizing the exergy consumption in WHENs compression and expansion should start at pinch, ambient, or hot/cold utility temperatures depending on the design problem. Furthermore, conditions for operating at these temperatures are described in the theorems. A manual design procedure was developed that use the insight provided by the theorems to design a work and heat exchange network with minimal exergy destruction. The procedure uses the heat cascade and Grand Composite Curve to locate the process pinch points and heat deficit above (and heat surplus below) the pinch points. The variable pressure streams are then added succesively to the network by splitting the streams and calculating the heat capacity flowrates for which the heat of compression (or cooling from expansion) exactly matches the heat available in the Grand Composite Curve. However, the procedure is iterative in nature and requires the designer to resolve the heat cascade and Grand Composite Curve for each variable pressure stream that is added. The procedure is tedious, to the point of being limiting even for smaller problems.

It should be mentioned that our approach to WHENs in this paper is not a truly simultaneous optimization procedure for Work and Heat Exchange Networks, since work integration is not included. Our focus is on utilizing the heating from compression and cooling from expansion in the heat recovery problem in order to reduce the consumption of thermal utilities by paying a small penalty in power. Integration of work between expanders (turbines) and compressors can be done directly (shaft work) or indirectly (power). Design of the work and power system (compressors, pumps, expanders, motors and generators) of a processing plant is a separate problem and can be addressed after solving the WHENs problem using the approach indicated in this paper. Finally, it should be mentioned that there is no "pressure Pinch" similar to the temperature Pinch.

A superstructure for WHEN synthesis was proposed by Uv[29] that accounts for the results from the theorems for correct integration of compressors and expanders in HENs. The superstructure splits the variable pressure streams into n stream branches, each with a different compression/expansion temperature. The superstructure is depicted in Figure 1 for a variable pressure stream undergoing compression. The integration of expanders is analogous. As seen from Figure 1, the pressure-changing units interact with the HEN through the set of individual heat exchangers placed both upstream and downstream of the compressors. Isothermal mixing is assumed in the superstructure, such that the individual target temperature for each of the stream branches should equal the target temperature of the parent stream. Furthermore, the supply temperature is equal for all the stream branches.[29] Therefore, each stream branch individually contributes to the heating or cooling of the process at different temperature levels. Allowing non-isothermal mixing would make the problem definition richer and the feasible solution space larger, however, at the expense of computational complexity. One option could be to run an NLP optimization for the network configuration found by the current model where the isothermal mixing assumption is relaxed. This is similar to what is done with the stage-wise superstructure by Yee and Grossmann[30] for HENs. The allocation of pressure changing equipment between Single Shaft Turbine Compressor (SSTC) units and utility compressor/expanders are not considered in the superstructure. Instead, this could be done during post-processing, or through an economic analysis.

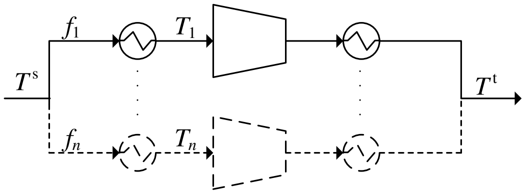


Figure 1: The WHEN superstructure for integration of compressors by Uv.[29]

Uv also developed an optimization strategy for the superstructure by emulating the manual design procedure.[29] Through pre-processing using the heat cascade, the process pinch points were located and used as compression and expansion temperatures in the stream branches. Additional stream branches with compression/expansion starting at the ambient temperature, and hot or cold utility temperatures were also included. Then a linear program was solved for finding the stream split distribution that yields a minimum exergy consumption. Similar to the manual design procedure, the optimization strategy is sequential in nature, where the process pinch points are first located prior to optimization, and then included in the superstructure as individual target temperatures for the stream segments upstream of the compressors/expanders. The problem therefore becomes that of exergy targeting with known supply and target temperatures, which can be solved using linear programming techniques. However, as explained by Vikse *et al.*,[31] the sequential approach suffers from several disadvantages such as inability to address (i) the optimal sequence of integration for compressors and expanders, and (ii) variable pressure specifications. The most important limitation, however, is that the creation of additional pinch points due to the integration of variable pressure streams, will lead to an iterative approach, where additional stream branches must be included as new pinch points occur. Alternatively, a simultaneous strategy similar to the approaches described by Wechsung *et al.*[14] and Nair *et al.*[18] can be employed. In that case, the target temperatures of the stream segments upstream of the compressors and expanders are treated as soft specifications and solved as part of the optimization problem. This requires the use of a simultaneous optimization and heat integration algorithm, and the disadvantage is that a nonconvex NLP model or an MINLP model will replace the much simpler LP model.[31]

Simultaneous optimization and heat integration algorithm by Duran and Grossmann

Two main methodologies for designing HENs exist in the literature. The first is the Pinch Design Method (PDM),[32] which is based on the concept of a heat recovery pinch, and relies on a manual design procedure. Although the PDM has achieved success in designing HENs, it suffers from inherent limitations regarding the problem size and considerations of economic trade-offs. Moreover, the method assumes fixed supply and target temperatures for the process streams, which is a limitation when integrating reactors and pressure changing equipment where temperatures should be regarded as part of the optimization problem.

Therefore, a second approach using Mathematical Programming has received increased attention. Different simultaneous optimization and heat integration models can be found in the literature, among them the formulations by Grossmann et al.,[21] Anantharaman *et al.*,[33] and Quirante *et al.*[22] In addition, a HEN synthesis model that handles variable stream temperatures has been developed by Yee and Grossmann[30] based on a superstructure approach in which every hot and cold stream is allowed to exchange heat over a predefined number of stages.

The first and perhaps best known simultaneous optimization and heat integration formulation was developed by Duran and Grossmann.[20] Similar to the PDM, their mathematical formulation is based on the concept of the process pinch, and in particular the decomposition that exists at this point, where there is a net heat deficit above, and a net heat surplus below the pinch point. The resulting optimization problem is presented in Equation (1).

$$\begin{aligned}\min_{\mathbf{x}} \quad & c_{\mathrm{CU}} Q_{\mathrm{CU}} + c_{\mathrm{HU}} Q_{\mathrm{HU}} \\ \text{s.t.} \quad & \sum_{i \in H} F_i (T_i^{\mathrm{s}} - T_i^{\mathrm{t}}) - \sum_{j \in C} f_j (t_j^{\mathrm{t}} - t_j^{\mathrm{s}}) + Q_{\mathrm{HU}} - Q_{\mathrm{CU}} = 0, \\ & z^p - Q_{\mathrm{HU}} \leq 0, \quad \forall p \in H \cup C, \\ & Q_{\mathrm{HU}} \geq 0, Q_{\mathrm{CU}} \geq 0,\end{aligned} \tag{1}$$

where z^p is defined by the following expression

$$\begin{aligned} z^p := & \sum_{j \in C} f_j [\max\{0, t_j^{\mathrm{t}} - (T^p - \Delta T_{\min})\} - \max\{0, t_j^{\mathrm{s}} - (T^p - \Delta T_{\min})\}] \\ & - \sum_{i \in H} F_i [\max\{0, T_i^{\mathrm{s}} - T^p\} - \max\{0, T_i^{\mathrm{t}} - T^p\}], \end{aligned} \tag{2}$$

and the pinch candidate temperatures T^p are provided by Equations (3) and (4) for hot and cold streams, respectively.

$$T^p = T_i^s, \quad \forall p = i \in H, \tag{3}$$

$$T^p = t_j^s + \Delta T_{\min}, \quad \forall p = j \in C. \tag{4}$$

The Duran and Grossmann formulation looks at all candidate pinch points T^p in the process and calculates the net heat deficit above each candidate. The first inequality constraint in Equation (1) then ensures that the minimum hot utility Q_{HU} can completely cover this net heat deficit. An additional energy balance for the process is included to calculate the resulting cold utility consumption Q_{CU}. The resulting model is a nonlinear program (NLP) where nonsmooth max operators are included to determine whether a process stream is located entirely above, across or entirely below the pinch candidate temperature. Consequently, there exist points of nondifferentiability where the Jacobian is undefined, which can cause problems for derivative-based solvers. Duran and Grossmann approached this issue by proposing the use of a smooth approximation such as the one suggested by Balakrishna and Biegler[34] for the max operator:

$$\max\{0, f(x)\} \approx \frac{\left(\sqrt{f(x)^2 + \beta^2} + f(x)\right)}{2}. \tag{5}$$

However, the selection of the user-defined parameter β is non-trivial and may lead to either an ill-conditioned approximation or loss of accuracy when poorly chosen.[21]

Nonsmooth analysis

Alternatively, there exist extensions to the concept of derivatives that are applicable to certain classes of nonsmooth functions. One such generalized derivative is the Clarke generalized Jacobian that is applicable to locally Lipschitz continuous functions.[35] A challenge with using elements of the Clarke Jacobian, however, is that these elements only follow calculus rules (e.g. the chain rule) as inclusions, which can be quite weak, and are therefore impractical to calculate for most complex composite functions. The lexicographic (L-)derivative is another generalized derivative for functions that satisfy the conditions for lexicographic (L-)smoothness as described by Nesterov.[36] The L-derivative was shown to be just as useful in nonsmooth numerical methods as elements of the Clarke Jacobian.[37] Furthermore, the authors developed an automatic differentiation framework for calculating these L-derivatives for composite functions by introducing a generalization of the directional derivative known as the lexicographic directional (LD-)derivative.[26] The LD-derivative is computed sequentially along the directions indicated by the columns of the directions matrix $\mathbf{M}$. Furthermore, it follows calculus rules as equations rather than as inclusions, and can therefore also be readily applied to composite functions. An extensive review on evaluating LD-derivatives and their applications is provided by Barton *et al.*[38]

Flowsheet optimization using LD-derivatives for sensitivity calculations have already been applied to liquefied natural gas (LNG) processes. A large temperature span from ambient temperature to approximately -160°C together with small temperature differences in the heat exchangers make natural gas liquefaction processes challenging to analyze. The small driving forces are a result of heat exchange at cryogenic temperatures where thermodynamic irreversibilities become significant. In particular, conventional state-of-the-art process simulators lack rigorous checks to avoid temperature crossovers in the multistream heat exchangers, and a feasible operating condition must therefore be determined through a manual iterative approach. Consequently, a simulation and optimization tool was developed using a nonsmooth flowsheeting strategy. The model includes a reformulation of the Duran and Grossmann model for preventing temperature crossovers.[25] Furthermore, additional nonsmooth equations are included for correct phase detection of the process streams.[39–42] The resulting model was simulated for single mixed refrigerant (SMR)[43] and dual mixed refrigerant (DMR) processes[44] using a nonsmooth Newton solver. Later, optimization was included using IPOPT as a solver. Despite assumptions of twice differentiable objective and constraints, IPOPT was shown to provide good results when using LD-derivatives for sensitivity information, as long as the dual feasibility criterion is relaxed.[45] Optimization was performed successfully for several SMR processes.[45]

Nonsmooth extension for unclassified process streams

The stream branches in Figure 1 interact with the HEN both upstream and downstream of the pressure-changing units through the individual heat exchangers. The compression/expansion temperatures can vary greatly in the model, where according to the theorems, compression/expansion should be carried out from the pinch temperature, ambient temperature, and hot or cold utility temperature depending on the design problem. In the sequential optimization procedure proposed by Uv,[29] the large span in possible compression/expansion temperatures does not present a modeling issue, as each candidate inlet temperature (i.e. pinch candidates, utility temperatures and the ambient temperature) is enumerated during pre-processing. Consequently, the stream classification can be fully determined for each compression/expansion temperature prior to optimization. However, in the simultaneous approach, each compression/expansion temperature is treated as a variable by the optimization model. The temperatures can therefore vary greatly, not only between different design problems, but also for each iteration step of the optimizer. Consequently, the classification of streams cannot be determined a priori in the superstructure.

Although the simultaneous optimization and heat integration algorithm by Duran and Grossmann[20] can handle variable supply and target temperatures, it assumes the stream classifications to be known. However, here we show that the algorithm can be extended to the problem of unclassified process streams by the inclusion of the nonsmooth Equations (6) and (7):

$$\begin{aligned} T_i^{\mathrm{s}} &= S_i^{\mathrm{s}}, \quad \forall i \in U, \\ T_i^{\mathrm{t}} &= \min(S_i^{\mathrm{s}}, S_i^{\mathrm{t}}), \quad \forall i \in U, \end{aligned} \tag{6}$$

$$\begin{aligned} t_j^{\mathrm{s}} &= S_j^{\mathrm{s}}, \quad \forall j \in U, \\ t_j^{\mathrm{t}} &= \max(S_j^{\mathrm{s}}, S_j^{\mathrm{t}}), \quad \forall j \in U, \end{aligned} \tag{7}$$

where U is the set of unclassified process streams, S_i^{s} and S_i^{t} are the supply and target temperatures of the actual stream, T_i^{s} and T_i^{t} are the supply and target temperatures of the hot substream, and t_i^{s} and t_i^{t} are the supply and target temperatures of the cold substream. Rather than using binary variables, the nonsmooth extension splits each unclassified process stream into a hot and cold substream, respectively. The supply temperature for each substream is set equal to the parent stream, whereas the target temperature is determined by Equations (6) and (7). Depending on the target temperature only one of the two substreams becomes active in the integration problem. For the case where the target temperature is less than the supply temperature, the unclassified process stream is in fact a hot stream, and the min operator in Equation (6) assigns the correct target temperature. The corresponding cold substream, on the other hand, is assigned by Equation (7) to a target temperature equal to its supply temperature. Consequently, it contributes neither to the overall energy balance nor to the energy balance above each pinch candidate (Equation (2)) and is therefore deactivated in the heat integration problem. The reverse becomes true if the unclassified stream behaves as a cold stream, when the target temperature is greater than the supply temperature. Figure 2 shows the target temperatures of the two substreams as a function of the target temperature of the parent stream. As can be seen from the figure, the hot (cold) substream only contributes to the overall heat integration problem, when the target temperature of the parent stream is less (higher) than the supply temperature of the substream.

Examples

Different examples are used to demonstrate the nonsmooth extension for heat integration with unclassified process streams. Examples are taken from the papers by Fu and Gundersen on the integration of compressors and expanders in above ambient networks.[10,11] Previously, these examples were solved using a manual design procedure for WHEN synthesis with the

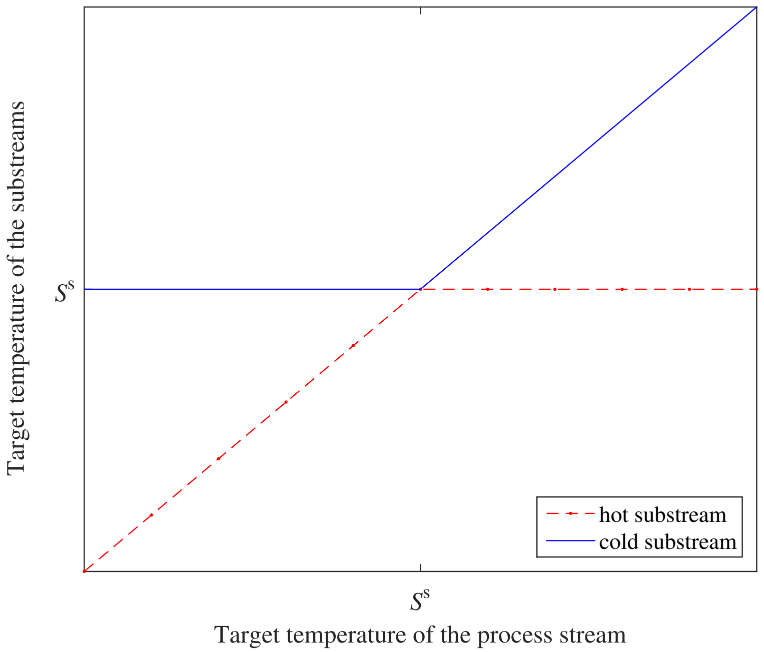


Figure 2: Target temperatures of the hot and cold substreams as a function of the target temperature of the parent stream.

objective of minimizing exergy losses. The procedure is iterative in nature, thus preventing the issue of unclassified process streams. In this article, the examples are solved using the WHEN superstructure from Uv[29] with the extended Duran and Grossmann formulation. The models are written in Julia v0.6.0 and run on a Dell Latitude E5470 laptop in the Ubuntu v16.10 environment with an Intel Core i7-6820HQ CPU at 2.7 GHz and 8.2 GB RAM. Optimization is done using IPOPT v3.12.6[27] with sensitivities provided by the generalized derivative elements. Similar IPOPT settings as proposed by Watson et al.[45] were used for solving the WHEN optimization problems. However, the maximum number of iterations was increased from 500 to 2000. Furthermore, the tolerance (here the dual feasibility tolerance) was increased to 1.0 due to empirical improvements to convergence for some instances. A full set of non-default IPOPT settings are provided in Table 1.

Table 1: Non-default settings for IPOPT used in this work.[45]

tol	1.0
constr_viol_tol	10^{-6}
bound_push	10^{-9}
bound_frac	10^{-9}
recalc_y_feas_tol	10^{-2}
max_iter	2000
mu_strategy	adaptive
hessian_approximation	limited-memory
limited_memory_max_history	number of decision variables

Assumptions and problem formulation

Different assumptions were made when deriving the theorems for appropriate placement of pressure-changing equipment.[11] Firstly, the supply and target temperatures must be known a priori, and remain fixed during optimization. In addition, the authors assume a single hot and cold utility at constant temperature. The variable pressure streams behave as ideal gases with a constant heat capacity ratio $\kappa \equiv c_p/c_v$, and the compressor/expander efficiencies are constant. As the theorems provide the foundation for the superstructure, the same assumptions are made for the examples in this article.

The maximum number of stream splits for the variable pressure streams is limited to three in the model to limit the problem size, and to prevent capital intensive solutions with large number of splits and low branch flowrates. Figure 3 shows the compression scheme for a variable pressure stream with three stream branches. The variables in the model are the individual branch heat capacity flowrates and temperatures, as well as the net work and hot/cold utility consumption.

As pressure changing equipment are included in the model, the objective from Equation (1) of minimizing hot/cold utility consumption is changed to that of minimizing the total exergy consumption:

$$Ex(\mathbf{x}) = Q_{\mathrm{HU}}(\mathbf{x}) \left(1 - \frac{T_0}{T_{\mathrm{HU}}}\right) - W_{\mathrm{net}}(\mathbf{x}), \tag{8}$$

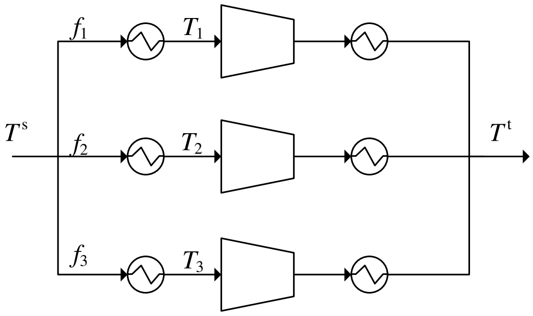


Figure 3: Superstructure for placement of compressors in HENs. The superstructure is analogous for expanders.

where T_{HU} is the hot utility temperature and T_0 is the ambient temperature, both in units of Kelvin, and $\mathbf{x}$ is a vector of the compression/expansion temperatures and heat capacity flowrates. The exergy of the cold utility is not included in the objective function as the cold utility temperature is equal to the ambient temperature, i.e., the reference temperature for exergy calculations, and thus the Carnot factor becomes zero. Furthermore, the superstructure assumes isothermal mixing at the outlet temperature T^{t}. The temperatures after compression/expansion are calculated using the following relation:

$$T_{\mathrm{out}} = T_{\mathrm{in}} \left(\frac{P^{\mathrm{t}}}{P^{\mathrm{s}}} \right)^{(\kappa - 1.0)/\kappa} . \tag{9}$$

As derivatives can readily be obtained for this function using the AD framework mentioned previously,[26] Equation (9) is included as a subroutine rather than an equality constraint resulting in fewer variables in the model. Consequently, outlet temperatures from compression/expansion are not independent variables in the optimization model. Instead, the temperatures as well as the sensitivities are calculated in the subroutine using the AD framework by Khan and Barton.[26] A heat capacity ratio of $\kappa = 1.4$, ambient temperature $T_0 = 15$°C, and a $\Delta T_{\min} = 20$ K are used in all the examples. Bounds on the optimization variables are provided in Table 2. The hot and cold utility duties are bounded from below to only take non-negative values. For the variable pressure streams, expansion and compression temperatures are bounded by the ambient and hot utility temperatures. In addition, the individual branch heat capacity flowrates are bounded between zero flow and the total heat capacity flowrate F of the variable pressure stream in question. Optimization is done from a starting point with compression/expansion temperatures of 400°C, 150°C and 100°C, and with branch heat capacity flowrates distributed equally.

Table 2: Variable bounds for the examples.

Variable	x_L	x_U	**Variable**	x_L	x_U
Q_{CU} [kW]	0.0	`inf`	Q_{HU} [kW]	0.0	`inf`
T_1	T_0	T_{HU}	T_2	T_0	T_{HU}
T_3	T_0	T_{HU}	f_1	0.0	F
f_2	0.0	F	f_3	0.0	F

Example 1: The first example is a heat integration problem taken from Fu and Gundersen,[11] where a hot stream undergoes an expansion from 2500 kPa to 100 kPa. Supply and target temperatures are fixed for all the streams, including the stream undergoing pressure change. Furthermore, utilities are assumed available at constant temperatures, specifically at 400°C and 15°C for hot and cold utilities, respectively. Stream data are provided in Table 3.

Table 3: Stream data for Example 1.

Stream	T^s [°C]	T^t [°C]	F [kW/°C]	P^s [kPa]	P^t [kPa]
H1	400	60	3	-	-
H2	400	280	2	2500	100
C1	200	380	8	-	-
Hot utility	400	400	-	-	-
Cold utility	15	15	-	-	-

As supply and target temperatures are fixed for the constant pressure streams, only hot stream H2 constitutes an unclassified process stream in this example. It is denoted as a hot stream in Table 3, merely for convenience since it has a target temperature lower than its supply temperature. Furthermore, since a stream split with three branches is used in the superstructure and each branch is represented by substreams both upstream and downstream of the expanders, there is a total of six unclassified streams in this example.

IPOPT obtained a solution to the WHENs problem after 28 iterations and a total CPU time of 3.2 s. Expansion should be done solely from the hot utility temperature, yielding a net exergy generation of 203.34 kW. The same solution was also obtained by Fu and Gundersen using the manual approach.[11] Table 4 shows the path of the two substreams S1 and S2 before and after expansion. As the expansion temperature is equal to the supply temperature of the variable pressure stream, no integration in the HEN is required upstream of the expander. Instead, the substream is expanded immediately to a temperature $T_{\text{ex}} = -4.80°\text{C}$. As the temperature from expansion (T_{ex}) is less than the target temperature, substream S2 must be heated and hence becomes a cold stream.

Table 4: Path of the variable pressure stream at the solution of Example 1.

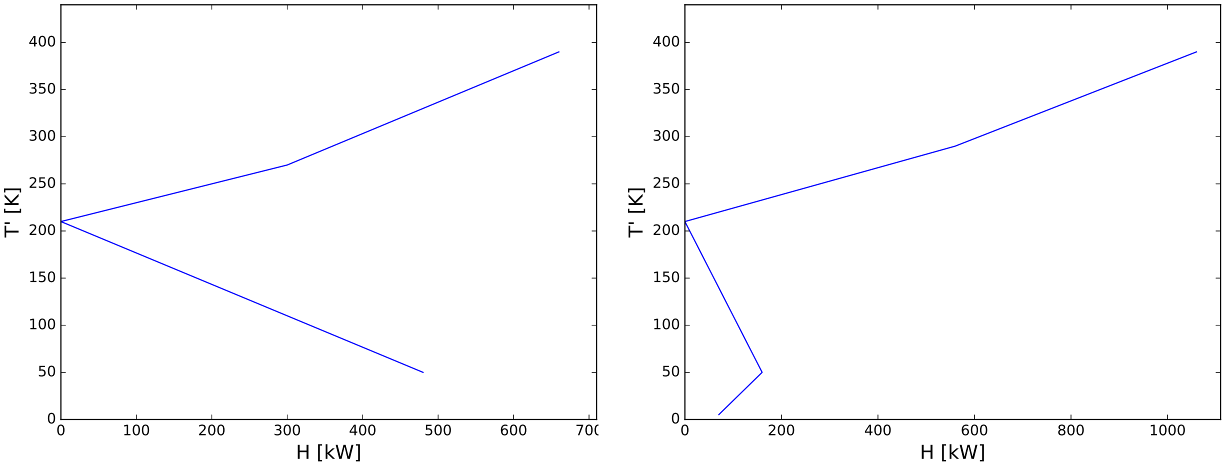
Stream	T^{s} [°C]	T^{t} [°C]	F [kW/°C]	P [kPa]	Classification
S1	400.00	400.00	2	2500	-
S2	-4.80	280.00	2	100	C

The hot and cold utility consumption, net work and total exergy consumption for the WHEN solution are presented in Table 5. The solution of the heat integration problem with no pressure manipulation is given for comparison. Expansion at the hot utility temperature increases the hot utility consumption from 660.00 kW to 1059.91 kW. Simultaneously, the necessary cold utility is reduced from 480.00 kW to 70.36 kW due to cooling from expansion. The net work from expansion is -809.55 kW, hence work is produced by the system. The pinch temperature remains the same for the HEN and WHEN. Furthermore, as the outlet temperature from expansion at hot utility temperature is lower than the ambient temperature, no pinch expansion is needed. Instead, IPOPT finds a solution where the variable pressure stream is expanded at the hot utility temperature directly. The Grand Composite Curves (GCCs) for the solution of (a) heat integration and (b) simultaneous work and heat integration problems are provided in Figure 4.

Example 2: This is an example taken from Fu and Gundersen[10] where a stream undergoes a pressure change from 100 kPa to 300 kPa. Stream data and utility temperatures are

Table 5: WHEN results and HEN targets without pressure manipulation for Example 1.

Property	**No pressure manipulation**	**WHEN solution**
Hot utility consumption [kW]	660.00	1059.91
Cold utility consumption [kW]	480.00	70.36
Pinch temperature [°C]	(220.00/200.00)	(220.00/200.00)
Net work [kW]	-	-809.55
Total exergy consumption [kW]	-	-203.34



(a)

(b)

Figure 4: (a.) Grand Composite Curve for Example 1 without pressure manipulation. (b.) Grand Composite Curve for the simultaneous work and heat integration problem.

presented in Table 6. As in the previous example, the problem has 8 continuous decision variables: the hot/cold utility consumption, compression temperatures and branch flowrates.

Table 6: Stream data for Example 2.

Stream	T^{s} [°C]	T^{t} [°C]	F [kW/°C]	P^{s} [kPa]	P^{t} [kPa]
H1	400	60	2	-	-
C1	15	250	1	100	300
C2	200	380	4	-	-
Hot utility	400	400	-	-	-
Cold utility	15	15	-	-	-

A solution was obtained by IPOPT after 43 iterations and 3.8 s of CPU time, corresponding to a total exergy consumption of 309.18 kW. Again, IPOPT converged to the solution predicted by the manual design procedure. Only one stream branch remains active, with heaters placed both upstream and downstream of the compressor. First, the stream is heated to the cold pinch temperature of 200.00°C (not known a priori), where it is compressed before being cooled to its target temperature. Consequently, the two substreams are classified by the optimizer as cold (S1) and hot (S2) streams in this case. Table 7 shows the complete path of the variable pressure stream.

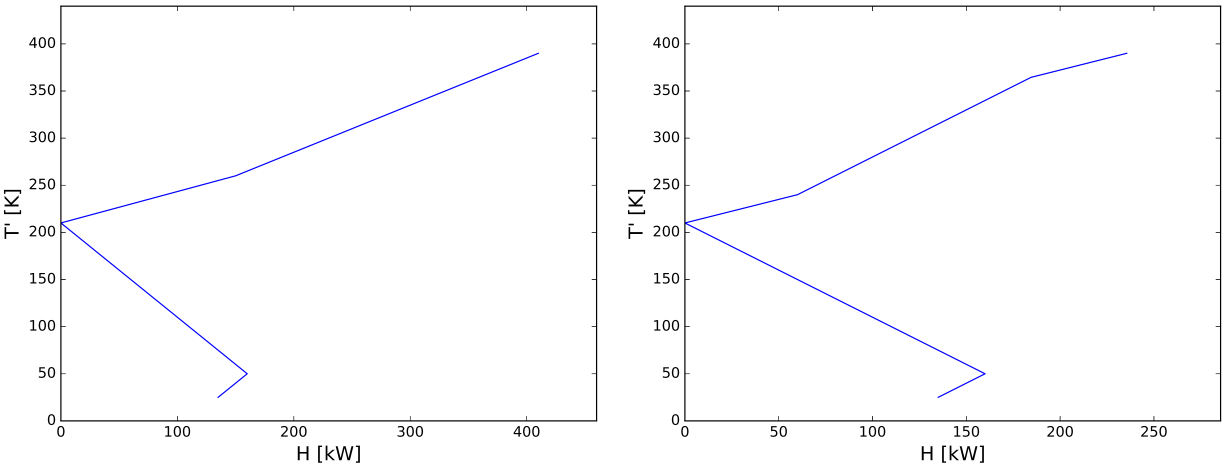
Table 7: Path of the variable pressure stream at the solution of Example 2.

Stream	T^{s} [°C]	T^{t} [°C]	F [kW/°C]	P [kPa]	Classification
S1	15.00	200.00	1.00	100	C
S2	374.49	250.00	1.00	300	H

The total exergy consumption, hot and cold utility consumption, and net work for the solution are presented in Table 8. The solution for the heat integration problem without pressure manipulation is presented in the same table for comparison. The example shows the trade-off between work and heat. Rather than cooling the stream prior to compression, the stream is heated (using surplus heat below pinch) to the pinch temperature, where it is compressed. Pinch compression provides additional heating above pinch, thus reducing the total required hot utility consumption. Consequently, through sacrificing some additional compression power due to a higher compression temperature, the total hot utility consumption in the network can be reduced. The GCCs for the two solutions are presented in Figure 5. The GCC for the WHEN is noticeably steeper above the pinch point due to compression. No additional pinch points are created in the WHEN solution, however, as the total heat from compression is less than the required heating at 374.49°C.

Table 8: WHEN results and HEN targets without pressure manipulation for Example 2.

Property	**No pressure manipulation**	**WHEN solution**
Hot utility consumption [kW]	410.00	235.52
Cold utility consumption [kW]	135.00	135.00
Pinch temperature [°C]	(220.00/200.00)	(220.00/200.00)
Net work [kW]	-	174.48
Total exergy consumption	-	309.18



(a)

(b)

Figure 5: (a.) Grand Composite Curve for Example 2 without pressure manipulation. (b.) Grand Composite Curve for the simultaneous work and heat integration problem.

Example 3: This is an example taken from Fu and Gundersen[10] integrating four streams; two hot and two cold, where a cold stream is compressed from 100 kPa to 300 kPa. The same example was used for demonstrating simultaneous optimization of work and heat integration with unclassified process streams in a paper by Yu *et al.*[19] In that article, an MINLP formulation was used to solve the problem, where the Duran and Grossmann formulation was extended to also account for unclassified streams by introducing binary variables. The resulting formulation contains a total of 168 continuous variables and 4 binary variables using the most compact of the formulations considered. Here the example is solved using the nonsmooth extension represented by Equations (6)-(7). As only one stream is compressed, the number of variables in the model is the same as for the previous two examples. Stream data is provided in Table 9.

Table 9: Stream data for Example 3.

Stream	T^{s} [°C]	T^{t} [°C]	F [kW/°C]	P^{s} [kPa]	P^{t} [kPa]
H1	300	50	4	-	-
H2	120	40	4	-	-
C1	70	380	3	100	300
C2	30	180	3	-	-
Hot utility	400	400	-	-	-
Cold utility	15	15	-	-	-

A solution with a total exergy consumption of 473.79 kW was obtained by IPOPT after 52 iterations and 3.9 s of CPU time. The path of the variable pressure stream for the two branches is presented in Table 10. Stream splitting is required here, with one stream branch (A) cooled down to 35.00°C where it is compressed and heated to target temperature. Stream branch (B), on the other hand, is first heated to the cold pinch temperature, and then compressed and cooled down to target. Consequently, the identity of both stream branches are different before and after compression. For comparison, the manual design procedure predicted identical exergy destruction and compression temperatures.

The optimization results are presented in Table 11, along with the results from heat integration only. If only heat integration is considered (no pressure manipulations in the network), the minimum hot and cold utility requirements are 360 kW and 300 kW, respectively. Provided a cold stream needs to be compressed from 100 kPa to 300 kPa, the heat of compression is sufficient to satisfy the heating demand from the process, hence resulting in

Table 10: Path of the variable pressure stream at the solution of Example 3.

Stream	T^{s} [°C]	T^{t} [°C]	F [kW/°C]	P [kPa]	Classification
Branch A:					
A1	70.00	35.00	1.53	100	H
A2	139.06	380.00	1.53	300	C
Branch B:					
B1	70.00	280.00	1.47	100	C
B2	483.63	380.00	1.47	300	H

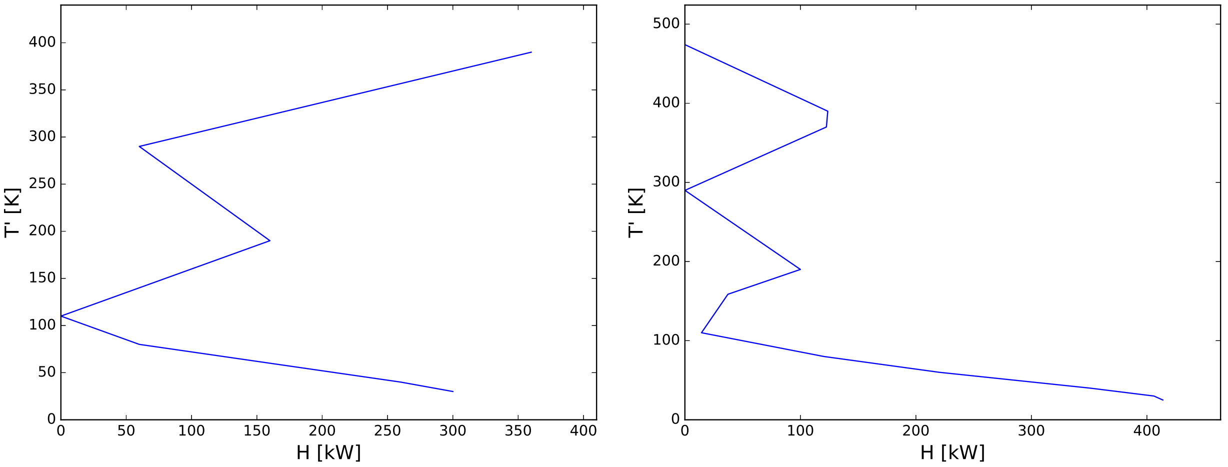
a threshold problem with no external hot utility consumption. Furthermore, the cold utility demand increases slightly from 300.00 to 413.79 kW from cooling stream branch A down to 35.0°C. Pressure manipulation results in two new pinch points at ($T_{\mathrm{H}}/T_{\mathrm{C}} = 484.12/464.12$°C) and ($T_{\mathrm{H}}/T_{\mathrm{C}} = 300.11/280.11$°C). GCCs for the WHEN solution and for the heat integration problem are presented in Figure 6.

Table 11: WHEN results and HEN targets without pressure manipulation for Example 3.

Property	**No pressure manipulation**	**WHEN solution**
Hot utility consumption [kW]	360.00	0.00
Cold utility consumption [kW]	300.00	413.79
Pinch temperature [°C]	(120.00/100.00)	(484.12/464.12), (300.11/280.11)
Net work [kW]	-	473.79
Total exergy consumption [kW]	-	473.79

Example 4: The example is taken from from Fu and Gundersen,[11] and is a work and heat integration problem with four process streams; two hot and two cold, where a hot stream needs to be expanded from 300 to 100 kPa. Detailed stream data are provided in Table 12.

IPOPT obtained a solution with a total exergy consumption of -206.18 kW after 53 iterations and 3.9 CPU seconds. At this solution, the stream branches A and B are active. As seen in Table 13, stream branch A is cooled down to the original hot pinch temperature at 330.02°C, expanded and further cooled down to target. Stream branch B is cooled down to 163.68°C, which is close to the new hot process pinch temperature 160°C, where it is expanded and reheated to the target temperature. Consequently, there is a stream classifi-



(a)

(b)

Figure 6: (a.) Grand Composite Curve for Example 3 without pressure manipulation. (b.) Grand Composite Curve for the simultaneous work and heat integration problem.

Table 12: Stream data for Example 4.

Stream	T^{s} [°C]	T^{t} [°C]	F [kW/°C]	P^{s} [kPa]	P^{t} [kPa]
H1	400	60	3	300	100
H2	330	80	9	-	-
C1	15	220	6	-	-
C2	140	380	8	-	-
Hot utility	400	400	-	-	-
Cold utility	15	15	-	-	-

cation change for branch B, where the stream is a hot stream upstream of the expander and a cold stream after.

Table 13: Path of the variable pressure stream at the solution of Example 4.

Stream	T^{s} [°C]	T^{t} [°C]	F [kW/°C]	P [kPa]	Classification
Branch A:					
A1	400.00	330.02	1.19	300	H
A2	167.52	60.00	1.19	100	H
Branch B:					
B1	400.00	163.68	1.81	300	H
B2	46.00	60.00	1.81	100	C

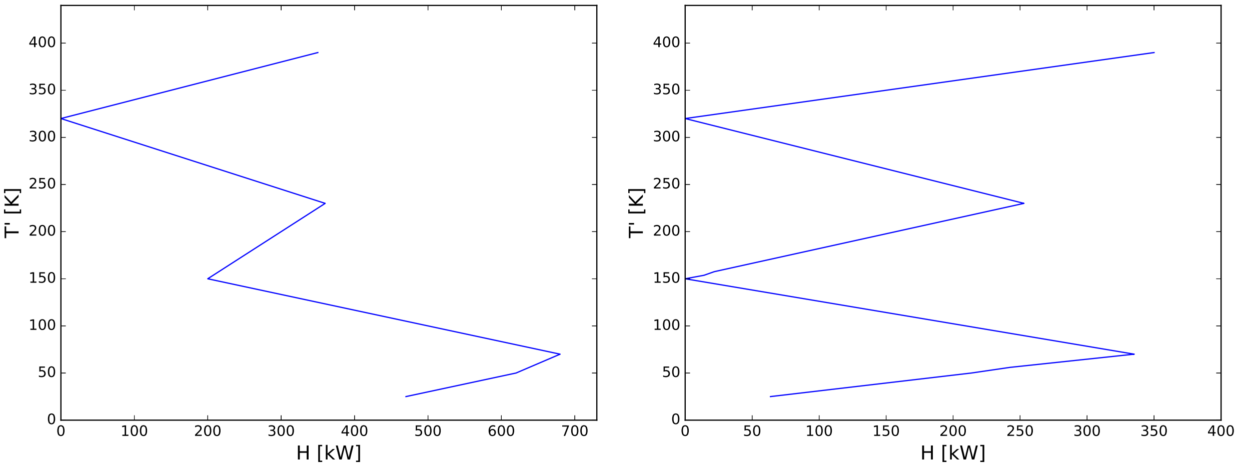
Table 14 presents the external utility consumption, net work and total exergy consumption for the optimized WHEN network. Pinch expansion reduces the required cold utility from 470 kW to 63.65 kW. Furthermore, it creates another process pinch point at ($T_{\mathrm{H}}/T_{\mathrm{C}}$ = 160/140°C) from pinch expansion at 330.02°C. The optimal solution with the manual procedure yields a total exergy consumption of -206.40 kW with expansion at the process pinch temperatures. The difference in objective function values is a result of expansion at a slightly higher temperature (163.68°C versus 160.00°C). IPOPT is run with a larger dual feasibility tolerance (see Table 1) due to the limitation of dual feasibility calculations being invalid at nonsmooth points, and hence convergence to suboptimal points is possible. A significant limitation with the manual design procedure is its iterative nature, which becomes very time consuming and even prohibitive for larger problems and several active stream branches. The authors analyzed this example also using the manual design procedure, experiencing the tediousness of the approach first hand. In particular, new heat cascades and GCCs must be calculated as each variable pressure stream is added to the network. If the heat from compression or cooling from expansion exceeds the required heating or cooling, stream splitting and several iterations are required for finding the optimal network. The optimization model, on the other hand, is simultaneous in nature, and will allocate the branch heat capacity flowrates between the different compression and expansion temperature candidates. Although the algorithm in some cases do not obtain the exact solution due to low tolerance for the dual feasibility calculations, it locates the correct pinch candidates for the integrated network, and suggests a compression or expansion scheme close to that of the manual procedure. Therefore, the algorithm is very suitable for speeding up the manual procedure, by first giving the designer a clear indication on which temperatures to compress and expand from. Then, the designer can use this information in the manual procedure, avoiding the iterative procedure for locating new pinch points, and determining the correct branch heat capacity flowrates. GCCs for the optimized WHEN and HEN are presented in Figure 7. The additional pinch point due to pressure manipulation can be seen in the figure. Additional cooling from expansion also makes the GCC noticeably steeper in the region below the high temperature pinch point.

Table 14: WHEN results and HEN targets without pressure manipulation for Example 4.

Property	**No pressure manipulation**	**WHEN solution**
Hot utility consumption [kW]	350.00	350.02
Cold utility consumption [kW]	470.00	63.65
Hot/cold pinch temperature [°C]	(330.00/310.00)	(160.00/140.00), (330.00/310.00)
Net work [kW]	-	-406.36
Total exergy consumption [kW]	-	-206.18

Example 5: The last example looks into the simultaneous compression and expansion of a hot and cold stream in a HEN. The example is taken from Fu and Gundersen[46] and looks at the integration of five streams; three hot streams and two cold streams. A hot stream undergoes a pressure change from 200 kPa to 100 kPa. Simultaneously, a cold stream needs to be compressed from 100 kPa to 200 kPa. With the simultaneous integration of two variable pressure streams, the total number of variables in the problem is 14. Stream data for the WHEN problem is provided in Table 15.

IPOPT obtained a solution after 135 iterations and 4.07 CPU seconds with a total exergy destruction of 175.89 kW. The paths of the two variable pressure streams are presented in Table 16. Each stream is split into two branches. Stream branch A of H1 is cooled down to a



(a) (b)

Figure 7: (a.) Grand Composite Curve for Example 4 without pressure manipulation. (b.) Grand Composite Curve for the simultaneous work and heat integration problem.

Table 15: Stream data for Example 5.

Stream	T^{s} [°C]	T^{t} [°C]	F [kW/°C]	P^{s} [kPa]	P^{t} [kPa]
H1	400	35	2	200	100
H2	320	160	4	-	-
H3	110	35	3	-	-
C1	15	380	3	100	200
C2	190	250	10	-	-
Hot utility	400	400	-	-	-
Cold utility	15	15	-	-	-

temperature 119.79°C where it is expanded and further cooled down to target. Branch B is expanded at a hot pinch temperature of 209.83°C. Similarly, stream branch A for cold stream C1 is compressed at a pinch temperature of 189.98°C, and then heated further to target. Stream branch B, on the other hand, is compressed at the pinch temperature 301.53°C and then proceeds to be cooled to target. The corresponding compression and expansion temperatures determined by the manual design procedure are 110.00, 210.00, 190.00 and 300.00 for the respective stream branches, resulting in a total exergy destruction of 175.6 kW.

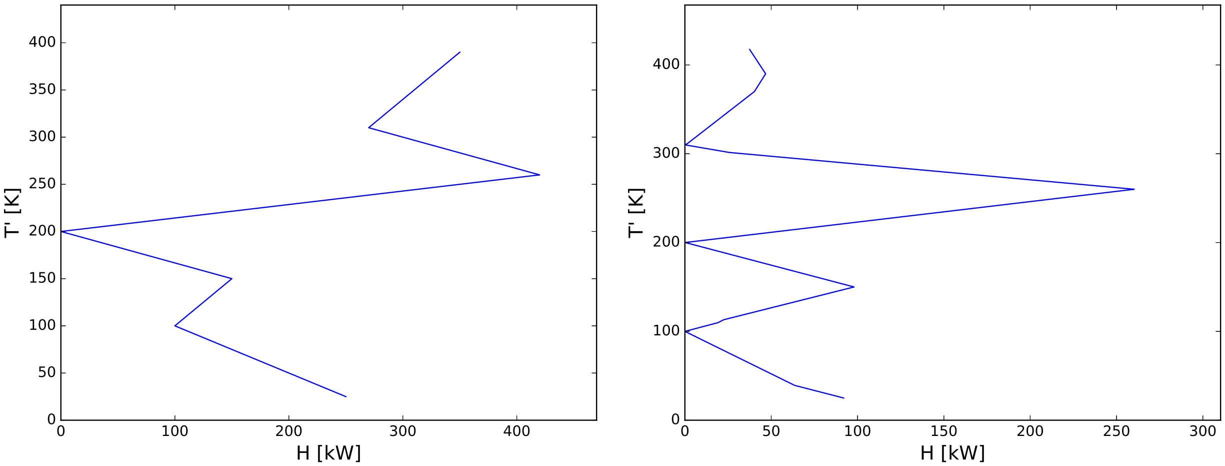
Table 16: Path of the variable pressure stream at the solution of Example 5.

Stream	T^{s} [°C]	T^{t} [°C]	F [kW/°C]	P [kPa]	Classification
H1:					
Branch A:					
A1	400.00	119.79	0.95	200	H
A2	49.19	35.00	0.95	100	H
Branch B:					
B1	400.00	209.83	1.05	200	H
B2	123.05	35.00	1.05	100	H
C1:					
Branch A:					
A1	15.00	189.98	2.66	100	C
A2	291.42	380.00	2.66	200	C
Branch B:					
B1	15.00	301.53	0.34	100	C
B2	427.40	380.00	0.34	200	H

The optimization results are summarized in Table 17. Heat from compression and cooling from expansion result in reduced hot and cold utility duties. Furthermore, additional pinch points are created at ($T_{\mathrm{H}}/T_{\mathrm{C}}$ = 110/90°C) and ($T_{\mathrm{H}}/T_{\mathrm{C}}$ = 320/300°C). The required net work for the process is 154.44 kW. GCCs for the HEN and WHEN are given in Figure 8.

Table 17: WHEN results and HEN targets without pressure manipulation for Example 5.

Property	**No pressure manipulation**	**WHEN solution**
Hot utility consumption [kW]	350.00	37.51
Cold utility consumption [kW]	250.00	91.95
Hot/cold pinch temperature [°C]	(210.00/190.00)	(110.00/90.00), (210.00/190.00), (320.00/300.00)
Net work [kW]	-	154.44
Total exergy consumption [kW]	-	175.89



(a)

(b)

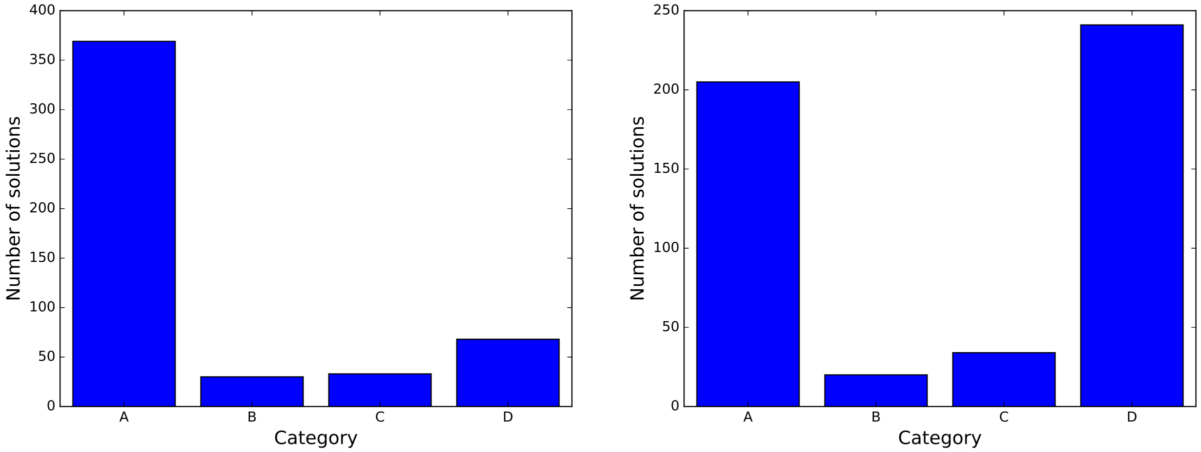
Figure 8: (a.) Grand Composite Curve for Example 5 without pressure manipulation. (b.) Grand Composite Curve for the simultaneous work and heat integration problem.

Convergence characteristics

Local optimization using IPOPT was used when performing the analysis. However, IPOPT assumes twice continuously differentiable objective function and constraints for the dual feasibility calculations. In particular, this creates an issue in defining the termination criterion for nonsmooth functions, as the dual feasibility calculations are invalid at nonsmooth points.[45] This can cause the algorithm to not converge, and instead iterate in a negligibly small search space. Here, this issue was resolved by increasing the dual feasiblity tolerance to 1.0. However, in order to avoid this issue completely, a new optimization solver tailored for handling L-derivatives must be developed. Nevertheless, solutions very close to the results from the manual design procedure were obtained in the examples. To investigate the performance of the local solver, multistart analysis were done for the five examples. The solutions were compiled into four main categories:

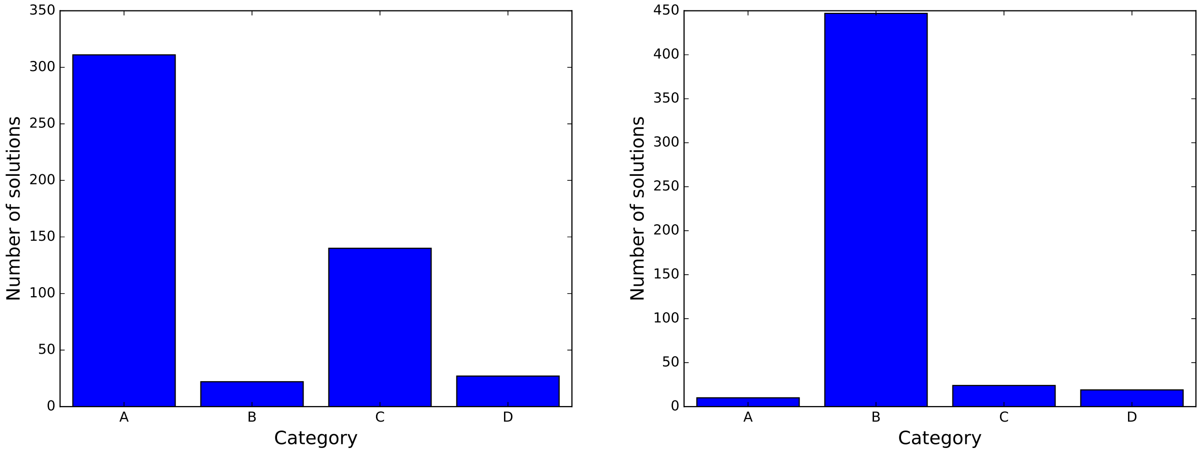
- A: Within 0.5% of the best known value.
- B: 0.5-2% of the best known value.
- C: 2-5% of the best known value.
- D: More than 5% of the best known value.

Multistart was performed by doing 500 runs and varying the initial guesses for the compression and expansion temperatures, which were varied in the ranges 15-100°C, 100-300°C and 300-400°C, respectively for the three stream branches. The results are given in Figure 9. The results show that IPOPT, although only a local algorithm, obtains the best known value or close to the best known value in most of the examples. Compressors and expanders add nonconvexity to the problem making it harder to achieve global convergence. However, even with the integration of two compressors and two expanders in Example 5, IPOPT still converges to solutions within 5% of the best known solution in 85% of the cases.



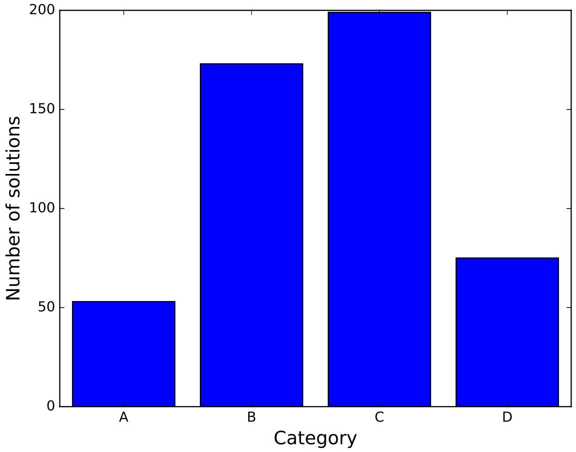
(a) Example 1.

(b) Example 2.



(c) Example 3.

(d) Example 4.



(e) Example 5.

Figure 9: Multistart results for the five examples.

The model needs to be tested for larger problems with more process streams, including streams that are subject to pressure change. The results from the five examples discussed in this paper are, however, quite promising when it comes to model performance. The required CPU times to solve these problems are really low, and only increases from 3.2 to 4.1 seconds when the number of streams increases from three to five. The number of pressure-changing streams increase from one to two.

Conclusions

A nonsmooth extension of the pinch location algorithm by Duran and Grossmann has been suggested for handling unclassified process streams. The extension uses the nonsmooth operators max and min for assigning target temperatures for streams of unknown classification. Streams that are inactive are given a target temperature equal to the supply temperature, and thus do not contribute to the overall energy balance in the model. Consequently, no binary variables are needed in the formulation, thus considerably reducing the computational efforts in solving the optimization model. The extension can be used both for the Duran and Grossmann formulation and the nonsmooth reformulation developed by Watson *et al.*[25] Examples are here done with the Duran and Grossmann formulation, as it was shown to provide better convergence characteristics. The extension was tested for five different work and heat integration problems of varying complexity using the local optimization algorithm IPOPT. Sensitivities for the nonsmooth operators are calculated analytically using recent developments in nonsmooth analysis and lexicographic directional derivatives. Solutions were obtained very close to the best known solution determined by a manual and iterative design procedure for all the examples. Furthermore, in several examples the solutions featured stream identity changes upon compression and expansion. Nonconvexity increases with additional streams in the problem, making it challenging to find global optima using only local solvers. Nevertheless, multistart analysis shows that IPOPT is still capable of finding good quality solutions even for the more complex examples. Future work will include embedding the models in a global optimization algorithm. The model should also be tested for cases with considerably more process streams.

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Nomenclature

Roman letters

C = Set of cold streams

$Ex(\mathbf{x})$ = Exergy consumption

F_i = Heat capacity flowrate of hot stream i [kW/K]

f_j = Heat capacity flowrate of cold stream j [kW/K]

f = Branch heat capacity flowrate [kW/K]

H = Set of hot streams

P = Pressure [kPa]

Q = Utility consumption [kW]

S = Temperature of the variable pressure stream [K]

T_0 = Ambient temperature [K]

T = Temperature of hot streams [K]

t = Temperature of cold streams [K]

U = Set of unclassified streams

W_{net} = Net work [kW]

Greek letters

ΔT_{min} = Minimum temperature difference [K]

κ = Heat capacity ratio

Subscripts and superscripts

CU = Cold utility

HU = Hot utility

i = Iteration variable for hot streams

j = Iteration variable for cold streams

L = Lower bound

p = Pinch candidate

s = Supply

t = Target

U = Upper bound

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Graphical TOC Entry