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A Generalized Approach to Handle Heat Exchange Restrictions in Energy Targeting

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This paper focuses on the development of a generalized method for describing and handling any type of heat exchange restrictions between subsets of thermal streams when dealing with automatic energy targeting. A graph theory representation of the heat exchange opportunities between stream subsets called heat integration graph is introduced. This graph is used to identify subsystems consisting of one or more stream subsets which can be treated as separate thermal cascades. These correspond to maximal subgraphs that are completely connected components of the heat integration graph, also called “cliques”. The stream subsets belonging to more than one clique, here called “pivot”, are those which thermal streams have to be optimally distributed to two or more cliques. The hot utility target of a system can then be found by solving a linear programming optimization in which the constraints that guarantee a feasible thermal cascade in all the maximal subgraphs are included. The procedure is applied here to a numerical example of a sugarcane mill in which some heat exchange restrictions are considered between process units.

1. Introduction

To generally address the analysis or the synthesis of heat exchanger networks, a graph theory approach is often used where process thermal streams are shown as nodes and heat exchangers are shown as edges. Since a heat exchanger is a valid match between a cold and a hot stream only and the direction of the heat transfer is also apparent, a heat exchanger network can be represented as a bipartite directed graph.
A similar representation is introduced in this work by looking at the process from a higher point of view that is by grouping process streams in subsets, for instance according to the way the streams appear in sub-processes. Stream subsets are represented as nodes and heat integration opportunities between stream subsets are shown with edges. Note that this type of graphs have no specific features as a stream subset can contain both cold and hot streams so the direction of the heat transfer between nodes is not known a priori and can vary between different temperature levels. Such graph theory representation is used here to facilitate and generalize the formulation of a mathematical procedure for estimating energy targets in systems where heat exchange restrictions appear between two or more subsets of thermal streams.
Energy targeting with conventional Pinch Analysis appears in fact less straightforward when dealing with heat exchange restrictions. Cascade calculations cannot take into account such constraints at once and more advanced analysis tools are therefore required. Although heat exchange restrictions can be easily taken into account in heat exchanger network synthesis (Papoulias and Grossmann, 1983), it is convenient to take into account their effects in energy targets without dealing with complex network synthesis in order to be able to compare system alternatives in a preliminary conceptual design phase.

1.1 Heat integration problems with restrictions

Pinch Analysis is typically used to analyze heat recovery potentials in systems where heat can be transferred between thermal streams without limitations (see Figure 1a). A relevant type of heat integration problem with restrictions where Pinch Analysis has been successfully applied is the case in which stream subsets can exchange heat only through an intermediate heat transfer medium such as a steam network

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(see Figure 1b). In this way better system energy targets are obtained than in the case the heat transfer is totally prohibited between the stream subsets but an energy penalty is introduced with respect to the case with no restrictions by larger temperature differences required for the intermediate heat transfer. Practical examples are large chemical processes or thermal power plants where heat recovery is impractical between some subprocesses far away from each other (Dhole and Linnhoff, 1992), or when heat integration is not possible between subprocesses that do not work simultaneously (Shang and Kokossis, 2004). Energy targets can be found in this case following the so-called total site methodology (Klemeš et al., 1997).

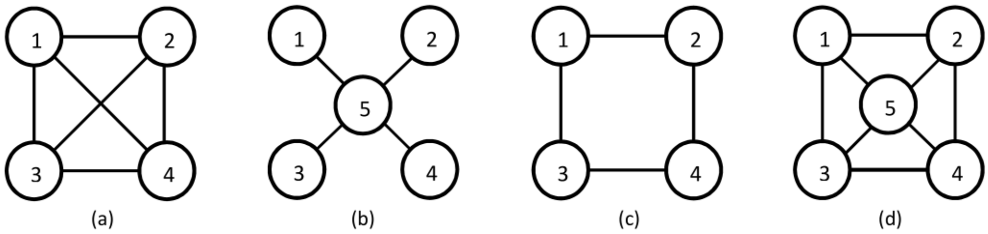

Figure 1: Examples of graph representation of heat integration opportunities between system stream subsets: (a) no heat exchange restrictions; (b) with heat exchange restrictions and total site stream subset; (c) with partial restrictions; (d) with partial restrictions and with total site stream subset

In the recent years different refinements of the total site methodology were suggested through combination of graphical and mathematical tools. For instance the graphical approach is combined with the study of the process utility matrix in (Nemet et al., 2012). Total site targeting with stream specific minimum temperature difference is proposed in (Fodor et al. 2012). Of particular interest is the application of integer and linear programming for optimizing the indirect heat transfer between the different stream subsets (Maréchal and Kalitventzeff, 1999). Heuristics are typically used to identify stream subsystems together with the set of thermal streams responsible for the indirect heat transfer between them resulting in a mathematical formulation of the heat integration problem that is often tailored to specific pattern of heat exchange restrictions. A more general mathematical formulation is proposed in (Becker and Maréchal, 2012) where heat exchange restrictions that allow to organize the heat integration in a hierarchy of progressively larger subsystems are investigated.

In the present work an attempt is made in the same direction by considering more complex restriction patterns than those commonly analyzed in the literature. In particular, a graph theory approach is proposed here for describing in similar way any kind of heat exchanger restriction patterns and for the automatic generation of algebraic constraints for the automatic solution of energy targeting problems.

Two examples of heat integration graphs are introduced in Figure 1c and 1d as opposed to the standard Pinch Analysis and total site cases. In Figure 1c direct heat exchange is possible between each subset and its “neighboring” subsets, e.g. between “1” and “2” and between “2” and “4”, but each subset has one “non-neighbor” with which heat cannot be exchanged, e.g. between “2” and “3” and between “1” and “4”. In Figure 1d the stream subset “5” can actually exchange heat with all the others and therefore used to achieve intermediate heat transfer between stream subsets which can however exchange heat directly to some extent.

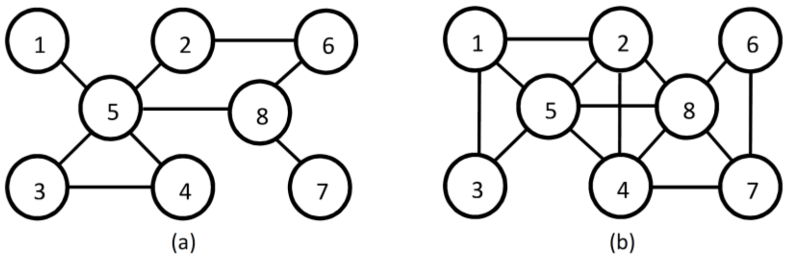

Figure 2: Examples of heat integration problems with complex patterns of heat exchange restrictions between subsets of thermal streams

In the examples in Figure 1c and 1d heat exchange restrictions do not allow treating any of the stream subsets, or sets of stream subsets, neither as completely separate subsystems nor as local subsystems with constant thermal cascade to which integrate a total site utility system. As a consequence the total site targets cannot be found just by algebraically evaluating separate thermal cascades and by finding the optimal distribution of a total site utility system only. Conversely the distribution of different stream subsets in different subsystems must be optimized simultaneously. In addition the hierarchical approach proposed in (Becker and Maréchal, 2012) appears of difficult application. The above simple examples open therefore the formulation of cases with rather complex restriction patterns as shown in Figure 2.

2. A generalized method for energy targeting with restrictions

The graphical solution of the constrained heat integration cases described above would require the simultaneous generation and modification of multiple stream subset grand-composite curves and would largely rely on heuristic choices. For this reason a mathematical approach is preferred. In particular, in the present work, the heat integration graph is used to study the heat exchange restrictions and to formulate constraints to be included in a mathematical optimization. To this end the maximal subgraphs are identified which correspond to subsets of stream subsets that can be treated as single thermal cascades in which pinch calculations can be made. As some stream subsets can participate to more than one maximal subgraph, the distribution of the thermal streams of such stream subsets is then optimized subject to the heat transfer feasibility constraints in each maximal subgraph cascade.

2.1 Maximal subgraphs

The graph theory formulation of heat integration between system stream subsets comes in help when looking at possible generalization of the above examples. The trivial case of Figure 1a where heat transfer between stream subsets can occur without restrictions (i.e. when a single global heat cascade is studied) can be characterized as a completely connected graph also denoted as K^n with n the number of stream subsets. Similarly, the case in which no heat transfer is admitted between stream subsets (i.e. n separate cascades are to be studied) corresponds to the empty edge set Ø.

The first functional characterization is introduced here by looking at the example in Figure 1b, the typical total site case. This case consists of four maximal subgraphs also called "cliques" that is completely connected subgraphs corresponding to subsets of stream subsets between which no heat exchange restriction appears. The following symbolic description can be given for the case in Figure 1b: {1,**5**};{2,**5**};{3,**5**};{4,**5**}. The four cliques share the same stream subset "**5**", shown in bold, which is called here as a "pivot" stream subset since its thermal streams may participate to four separate cascades. The other stream subsets of a clique contributing entirely and uniquely to the heat cascade of a single clique are instead referred to as "local".

This graph theory approach is particularly useful when the heat transfer is only partially admitted between subsets of thermal streams. In the example in Figure 1c, the symbolic formulation of the site heat integration graph is: {**1**,**2**};{**2**,**4**};{**3**,**4**},{**1**,**3**}. Unlike the case in Figure 1c where a single "pivot" stream subset appears, all the stream subsets are pivoting in this case. This means that none of the stream subsets contributes with a constant share to any clique and all stream subsets feature a partially restricted behavior.

The following symbolic formulations result for the other examples in the above pictures:

Figure 1d: {**1**,**3**,**5**};{**1**,**2**,**5**};{**2**,**4**,**5**};{**3**,**4**,**5**}, all subsets are pivot.

Figure 2a: {1,**5**};{3,4,**5**};{**2**,**5**};{**2**,**6**};{**5**,**8**};{**6**,**8**};{7,**8**}, unit "1", "3", "4" and "7" are local.

Figure 2b: {**1**,**5**,3};{**1**,**5**,**2**};{**2**,**4**,**5**,**8**};{**4**,**8**,**7**};{6,**7**,**8**}, unit "3" and "6" are local.

It is worth noting that a large number of stream subsets and multiple heat transfer restrictions can quickly complicate the identification of the maximal subgraphs and the observation of the heat integration graph might not be of sufficient help. To this end, algorithms can be used for identifying the maximal subsystems which can also be translated in computer code and used as a part of an automatic tool for energy targeting. Among several algorithms developed for this purpose in the past the Bron-Kerbosh algorithm is widely used (Bron and Kerbosch, 1973).

2.2 Translating maximal subgraphs in optimization constraints

When the load or the temperatures of one or more thermal streams in a system are to be adjusted according to a given objective, it is convenient to use the Pinch Analysis problem table to formulate the heat transfer feasibility constraint (the condition of minimum temperature difference between heat sinks and sources) as a set of inequality constraints. In fact, at each temperature interval, the balance between net heat cascaded from the interval immediately above and the net heat resulting from the balance of the interval hot and cold streams must be positive or equal to zero (in the latter case a pinch point activates).

Each maximal subgraphs of a given heat integration graph represent in fact a thermal cascade to which associate a set of inequalities constraints imposing a positive net heat load at each temperature interval to

guarantee the heat transfer feasibility. Once maximal subgraphs are identified, simple set operations are used to sort out the “local” stream subsets from the “pivot” stream subsets. The thermal streams belonging to these latter stream subsets are those which contributions to different cliques (thermal cascades) have to be decided. Conversely, local stream subsets participate as a constant term in their clique cascade.
The formulation of the heat integration problem in case of restrictions therefore differs from the unrestricted heat integration case by the only fact that a larger set of heat transfer feasibility inequalities is built by concatenating the inequalities related to the temperature intervals appearing in separate maximal subgraph cascades. Ultimately the hot utility target of a given system is estimated by deciding how the thermal streams of the pivot stream subsets should distribute to their cliques. In this work it was assumed that each stream of a pivot stream subset can be split in parallel (i.e. in multiple streams with the same inlet and outlet temperatures) to any of its cliques. In this case it is possible to use linear programming where linear variables x are associated to the portions of each thermal stream of each pivot stream subset p that contributes to each separate clique c.

Accordingly, for each clique c, given Lc local subsets and Pc pivot subsets, the heat transfer feasibility for a temperature interval u is generally expressed as:

$$R_{c,u} = \sum_{l}^{Lc} \sum_{i} q_{l,u}^{i} + \sum_{p}^{Pc} \sum_{h} (x_p^h \cdot q_{p,u}^h) + R_{c,u-1} \geq 0 \qquad (1)$$

where q is a stream heat load with its sign, and i and h are indexes of thermal streams respectively for local stream subset l and of a pivot stream subset p. Given C cliques, the system total heat demand is $Q = \sum_{c}^{C} R_{c,u=0}$. The system hot utility target is therefore estimated by solving the linear programming problem with the objective $\min Q = f(\bar{x}_p^h)$ subject to the constraints in Eq(1) written for all the temperature interval u for all the clique c.

3. Numerical example

The method is applied to a case study of a sugarcane plant for combined sugar and ethanol production. A process description together with a list of thermal streams is given in (Morandin et al., 2011). This example is used here only for clarifying the procedure for estimating the hot utility target given heat exchange restrictions between stream subsets, the discussion of its technological relevance being beyond the scope of this paper. Figure 2 provides the heat integration graph of the system used for the example.

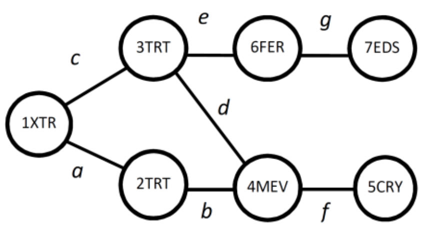

Figure 2: Heat integration graph for the sugarcane conversion plant example.

There are in total 41 thermal streams which are grouped in stream subsets according to the plant layout. The stream subsets are here labeled as follows: 1XTR: juice extraction (2 thermal streams); 2TRT: juice treatment to sugar (5 thermal streams); 3TRT: juice treatment to ethanol (5 thermal streams); 4MEV: five-effect evaporator (15 thermal streams); 5CRY: crystallization and drying (7 thermal streams); 6FER: must fermentor (2 thermal streams); 7EDS: ethanol distillation (5 thermal streams).
The heat integration is studied under the condition of minimum temperature difference of 4 °C. Under the hypothesis that heat transfer is allowed between all the stream subsets without restrictions, the process hot utility demand amounts to 100.6 MW (Morandin et al., 2011).
Heat transfer restrictions are now introduced between some process stream subsets and the system energy targets are calculated with the proposed procedure. In particular it is assumed that heat cannot be transferred between the stream subsets involved in the sugar production and those involved in the ethanol production with the only exception for the multi-effect evaporator. In addition, the distillation stream subset can be integrated only with the fermentor and the fermentor only with the treatment 3TRT. Further

restrictions are introduced so that crystallization and drying can be integrated only with the evaporator, and the juice extraction only with the treatment units. The following 7 maximal subgraphs (cliques) are identified: *a* {**1XTR**,**2TRT**}; *b* {**2TRT**,**4MEV**}; *c* {**1XTR**,**3TRT**}; *d* {**3TRT**,**4MEV**}; *e* {**3TRT**,**6FER**}; *f* {**4MEV**,5CRY}; *g* {**6FER**,7EDS}. Note that, in this particular case study, cliques correspond to graph edges as there are no maximal subgraphs with more than two stream subsets. Most of the stream subsets are of the pivot type, the stream subsets 5CRY and 7EDS being the only of local type respectively in clique *f* and *g*.

The hot utility target is found by solving a linear programming problem in which the objective function consists of the sum of the hot utilities of the 7 separate cliques. A total of 78 decision variables are used to optimize the distribution of the pivot thermal streams. Since the portions of each pivot stream must add up to the total stream heat load, 29 equality constraints are imposed being this the total number of streams of pivot stream subsets. By concatenating the heat transfer feasibility inequalities of the 7 separate clique cascades, a total of 336 inequalities result. The problem was solved using the Matlab embedded Simplex solver.

Table 1. Optimal distribution of thermal streams for the example of constrained heat integration of the sugarcane conversion plant.

Pivot stream subset	Tin (°C)	Tout (°C)	load to *a* (kW)	load to *b* (kW)	load to *c* (kW)	load to *d* (kW)	load to *e* (kW)	load to *f* (kW)	load to *g* (kW)	Total load (kW)
1XTR	50	25	726	-	0	-	-	-	-	726
	50	25	5,805	-	0	-	-	-	-	5,805
2TRT	98	97.9	3,263	0	-	-	-	-	-	3,263
	98	25	434	0	-	-	-	-	-	434
	73	72.9	0	478	-	-	-	-	-	478
	73	25	41	0	-	-	-	-	-	41
	39	105	0	28704	-	-	-	-	-	28,704
3TRT	98	97.9	-	-	1419	0	0	-	-	1419
	98	25	-	-	189	0	0	-	-	189
	73	72.9	-	-	208	0	0	-	-	208
	73	25	-	-	18	0	0	-	-	18
	39	105	-	-	0	12,446	0	-	-	12,446
4MEV	115	114.9	-	7,7038	-	16,964	-	0	-	94,002
	115	25	-	0	-	15,840	-	0	-	15840
	108	107.9	-	5,522	-	0	-	13749	-	19,271
	108	25	-	0	-	2,933	-	0	-	2,933
	98	97.9	-	0	-	10,392	-	10591	-	20,983
	98	25	-	0	-	2,773	-	0	-	2,773
	84	83.9	-	0	-	22,200	-	0	-	22,200
	84	25	-	0	-	2,287	-	0	-	2,287
	58	57.9	-	6,524	-	0	-	18891	-	25,415
	58	25	-	0	-	1,293	-	0	-	1293
	115	115.1	-	101,220	-	0	-	0	-	101,220
	108	108.1	-	0	-	17,492	-	0	-	17,492
	98	98.1	-	18,449	-	652	-	0	-	19,101
	84	84.1	-	19,976	-	0	-	0	-	19,976
	58	58.1	-	22,433	-	0	-	0	-	22,433
6FER	93	28	-	-	-	-	0	-	12549	12,549
	28	27.9	-	-	-	-	4,723	-	0	4,723

As a result, a hot utility target of 158.7 MW was obtained which corresponds to around 57 % increase with respect to the target of base case in which no heat exchange restrictions are. The values of the decision variables are shown in Table 1.

The results show that only 5 streams of the evaporator must be split to different cliques to minimize the process hot utility demand while the remaining 24 streams participate with their total load to single cliques. This optimal distribution of the thermal streams must be nevertheless interpreted as a result of the specific LP solver used. It is apparent that the multiple stream splitting solutions can lead to the same target being the objective function (the total process hot utility) insensitive to the way the streams are split until pinch points are activated in clique cascades. Lagrange multipliers may be studied in order to identify which streams activate a pinch point and in which cliques.

4. Conclusions

A graph theory approach is introduced in this work to generalize the mathematical formulation and solution of energy targeting problems in which heat exchange restrictions appear between subsets of thermal streams. The key aspect of the proposed method is the identification of the maximal subgraphs, also called “clique”, that is completely connected components of the heat integration graph which can be regarded as a separate thermal cascade that can be treated with the conventional Pinch Analysis problem table. This approach allows automatically identifying the “pivot” stream subsets which stream must be optimally split and distributed to multiple cliques to minimize the total system hot utility subject to the heat transfer feasibility each maximal subgraph thermal cascade. With respect to other methods presented in the literature for the solution of similar problems, the proposed approach allows formulating in an automatic way any pattern of the heat exchange restrictions between stream subsets as a set of algebraic inequality constraints given the site heat integration graph. Future applications of the present approach are planned for the analysis of primary energy saving opportunities in large refinery and petrochemical plants where the current heat exchanger networks and utility systems can be retrofitted to take better advantage of local and total site heat integration.

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