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# Energy Integration of Industrial Batch Processes (PinchBATCH) - Phase 2

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# ABSTRACT


A comparative study has demonstrated that the formerly developed Pinch Analysis (PA) based targeting and design methods outperform (in both heat recovery and cost-effectiveness) the simplified combinatorial design methods proposed by other authors (namely the Omnium Verfahren and the Permutation Method). The PA based methods provide valuable insight in the problem, but aren't suitable for automated design and optimization.
PinchBATCH results therefore in the following advances: **1)** a strategy (including guidelines and quantitative criterias) is proposed to restrict the analysis of batch processes to meaningful time slices. Likely variations of the schedule are taken into account; **2)** practical constraints limiting the repipe and resequence of heat exchangers are identified and formalized under a matrix format. The formalization of all these constraints is needed for automated design methods to actually focus on feasible solutions; **3)** a strategy based on genetic algorithms (GAs) is proposed for the synthesis of direct batch heat exchangers networks (i.e. without heat storage). The strategy features a decomposition into an upper level, which optimizes the overall network, and a lower level which search for the best use of the heat exchangers across time slices; **4)** for indirect heat recovery using heat storage, a heuristic, PA inspired approch for targeting and simplified design is proposed and demonstrated. It uses TAM composites and includes a method to identify the minimum number of heat storage units (HSUs) as function of the heat recovery. Most generally, local minimums are to be found just before a storage pinch appears, and the search strategy systematically removes one bottleneck at a time, taking advantage of the available degrees of freedom. A simple graphical tool to assess opportunities to decrease the required capacity of HSUs by rescheduling of streams is proposed. A model suitable for a GA based optimization is also proposed, featuring a decomposition into two levels; **5)** detailled specifications of the organization and of the features to be implemented in a software tool to address the heat integration of batch processes have been produced.

The very next steps will be concerned with the implementation and the validation of the GA based synthesis approaches.



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# RÉSUMÉ

Une étude comparative a démontré que les méthodes de *targeting* et de *design*, précédemment développées et basées sur l'analyse pincement (PA), surpassent - en potentiel de récupération de chaleur et en performances économiques - les méthodes de conception combinatoires simplifiées que sont la méthode Omnium et celle des Permutations. Les méthodes basées sur la PA permettent une compréhension approfondie du problème, mais ne sont pas adaptées au *design* automatique et à l'optimisation de réseaux.

PinchBATCH a ainsi permis les développements suivants: **1)** une stratégie (comprenant des recommandations et des critères quantitatifs) est proposée afin d'identifier les tranches de temps réellement significatives. Les variations probables de *schedule* sont prises en compte; **2)** les contraintes pratiques limitant le *repipe* et le *resequence* d'échangeurs de chaleur sont identifiées et formalisées sous forme de matrices de compatibilité. La formalisation des multiples contraintes est nécessaire pour que les méthodes de *design* automatique fournissent des solutions réalistes; **3)** une stratégie basée sur les algorithmes génétiques (GAs) est proposée pour la synthèse de réseaux d'échangeurs directs (c.-à-d. sans stockage de chaleur). La stratégie comprend une décomposition du problème en deux niveaux, le réseau global étant optimisé au niveau supérieur, tandis que l'usage optimal des échangeurs sur les différentes tranches de temps est recherché au niveau inférieur; **4)** une méthode heuristique basée sur la PA est proposée pour le *targeting* et le *design* simplifié de réseaux de récupération de chaleur avec stockage. Elle utilise les composites TAM et comprend une méthode pour déterminer le nombre minimum de stockages (HSUs) en fonction de la quantité de chaleur récupérée. Des minimums locaux résultent très souvent de l'apparition subite de pincements de stockage, et la stratégie consiste à éliminer les *bottlenecks* un à un, en mettant à profit les degrés de liberté à disposition. Une représentation graphique simple permet d'évaluer rapidement les opportunités de réduire le volume de stockage par *rescheduling* de flux. Un modèle mathématique adapté à une optimisation par GAs est également proposé; l'optimisation recourt à une décomposition en deux niveaux; **5)** des spécifications détaillées ont été produites concernant les fonctionnalités à implémenter dans un outil logiciel destiné à l'intégration de procédés discontinus.

La prochaine étape consistera à implémenter et valider les méthodes de synthèse automatique basées sur les GAs.

# ZUSAMMENFASSUNG

Eine vergleichende Studie zeigt auf, dass die vormals entwickelte Pinch-Analyse (PA) die von andern Autoren vorgeschlagene einfache, kombinatorische Designmethode (nämlich das Omnium-Verfahren und die Permutationsmethode) an Leistungsfähigkeit übertrifft. Methoden, die auf einem PA-Ansatz beruhen, geben zwar wertvolle Einblicke in das Problem, sind jedoch ungeeignet für ein automatisiertes Entwerfen und Optimieren. Durch PinchBATCH resultieren folgende Fortschritte: **1)** die vorgeschlagene Strategie beschränkt die Analyse der Batch-Prozesse auf sinnvolle Zeitabschnitte. Wahrscheinliche Änderungen des Zeitablaufs sind berücksichtigt; **2)** praxisbedingte Zwänge, die ein Wiederanschliessen von Wärmeaustauschern limitiert, werden aufgezeigt und in Matrixform dargestellt. Der Formalisierungsvorgang all dieser Zwänge ist notwendig für eine automatisierte Designmethode, die sich auf das Aufzeigen von realisierbaren Lösungen beschränkt; **3)** es wird eine auf genetischen Algorithmen (GA) beruhende Strategie zur Synthese von Wärme-austauscher-Netzwerken im Direktbetrieb (d.h. ohne Wärmespeicherung) aufgezeigt. Dieses Vorgehen bewirkt eine Dekomposition des Systems in eine obere Ebene, in der das Gesamtnetzwerk optimiert wird und eine untere Ebene, wo nach der besten Anwendung der Wärmeaustauschern bezüglich des Zeitplans gesucht wird; **4)** für eine indirekte Wärmerückgewinnung, die die Wärmespeicherung einsetzt, wird ein heuristischer, durch die PA inspirierter Lösungsansatz für Targeting und vereinfachten Entwurf vorgeschlagen. Dieser Lösungsansatz benutzt TAM-Verbundkurven sowie eine Methode zur Bestimmung der Minimalzahl von Wärme-speichereinheiten (HSU), die ihrerseits von der Wärmerück-gewinnung abhängig ist. Lokale Minima finanzieller Art befinden sich im allgemeinen stets vor dem Erscheinen von Speicher-Pinch's und die Suchstrategie eliminiert jeden einzelnen Engpass indem die verfügbaren Freiheitsgrade ausgenutzt werden. Es wird ein einfaches, grafisches Werkzeug zur Beurteilung der Möglichkeiten zur Senkung der benötigten HSU-Kapazität durch ein Wiedereinplanen der Ströme, vorgeschlagen. Dazu wird ebenso ein auf dem GA basierendes Modell erarbeitet, bei dem die Dekomposition der Optimierungsaufgabe in zwei Ebenen vorkommt; **5)** für SW-Tools, die geeignet sind zur die Energieintegration von Batch-prozessen, wurden Funktionalitätenbeschreibungen generiert.

Als nächster Schritt ist die Implementation und Evaluation von auf GA basierenden Lösungsansätzen vorgesehen.

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# Chapter 1

# EXECUTIVE SUMMARY

## 1.1 Context and Objectives

PinchBATCH has been initiated as the continuation of a former project (Krummenacher & Favrat, 1995) which has developed Pinch Analysis (PA) based procedures for the supertargeting of direct batch heat exchanger networks (HENs), as well as for the design and optimization of indirect heat recovery using intermediate heat storage. The performances of these procedures were demonstrated using simple example problems; both energy and cost savings achieved using heat storage were highlighted. The design, by hand, of an overall HEN able to operate feasibly within each time slice has been experienced as difficult and time consuming. Apart from simplified combinatorial methods such as the Omnium Verfahren (OV) and the Permutation Method (PM), the literature review (refer to *Appendix A*, and to Krummenacher & Auguste, 1997) has shown that more general, automated synthesis methods for batch HENs are not available. Heat integration methods focus either on the direct heat exchanges, or on the indirect heat recovery (HR), but seldom address the case of mixed direct-indirect heat integration.

The objectives of the PinchBATCH project have been defined as:

1. applying the formerly developed, Pinch Analysis based, supertargeting and design procedures on two industrial batch processes;
2. comparing the proposed Pinch Analysis (PA) approach with more design oriented combinatorial methods, namely the Omnium Verfahren (OV) and the Permutation Method (PM);
3. improving the supertargeting procedures;

4. proposing an automated or semi-automated methodology for the design and optimization of batch heat exchanger networks (batch HENs);
5. implementing the developed tools and methods in the PinchLENI software.

PinchBATCH has progressed in two phases (Phase 1 and Phase 2). The core of the present final report is concerned with Phase 2. Only the main results of Phase 1 (Krummenacher & Auguste, 1997 - available from ENET, Order Nr. 9655360) are summarized below.

### 1.1.1 PinchBATCH - Phase 1

Phase 1 has addressed the objectives 1, 2 and partly 5 mentionned above.

The comparisons of the Pinch Analysis (PA) based methodology with the Omnium Verfahren (Hellwig & Thöne, 1994) on the one hand, and with the Permutation Method (Stoltze *et al*, 1992, 1995) on the other hand, have been based on simplified example processes, which do not necessarily reflect industrial processes.

This choice was necessary since the analysis of the two industrial processes - a brewery (Krummenacher, 1995) and a multiproduct polymer resins plant (Cretegny, 1997) - revealed that these processes could not be used as they were. The brewery process included methodological difficulties to be overcome first (e.g. hot process water needs which were soft both in terms of time and temperature, varying process schedule). The polymer resins plant has revealed very little scope for heat recovery as it was, and no scope for beneficial process modifications since the processes were already certified and because the solvent imposed major constraints for safety and health reasons.

As far as the PinchLENI software is concerned, it has been noticed that the scope for implementing the proposed tools and methods was actually very limited. The PinchLENI Java project has been launched with the objective to restart on a new basis (both the language and data structures), so as to avoid the shortcomings observed in the existing PinchLENI. Minor additional features have been introduced in PinchLENI, while a significant amount of time has been devoted to the specifications of the data structures and the features of the new Java version.

## 1.1.2 PinchBATCH - Phase 2

From the overall objectives of the PinchBATCH project, objectives 3, 4 and part of 5 remained to be addressed after Phase 1 had been completed.

Phase 1 has stressed the need for automated design procedures and highlighted various practical constraints (e.g. schedule variations, re-use of heat exchangers) which should be taken into account in order for the developed methodologies to be meaningful in practice. Objective 3 (improving existing supertargeting procedures for direct heat integration) lost part of its relevance in this context, while the following aspects have received due consideration:

- the further development of the PA based design methodology for indirect heat recovery, given the significance of this mode of integration;
- a closer look at the practical constraints limiting the re-use of heat exchangers, i.e. distinguishing batch processes from multiple base cases (MBC) defined for flexible continuous processes;
- a review of the automated procedures for the design and optimization, and the search for models suitable for use with a genetic algorithm (GA) based optimization;
- various aspects such as "reduced" economic parameters, simple tools to assess rescheduling opportunities, etc.;
- not to forget the time consuming activity around LENIpass (i.e. the new PinchLENI software in Java).

Energy conscious engineers in the batch industry have shown interest in the proposed heat integration methodologies. Opportunities to apply these for a preliminary heat integration study of pigments manufacturing processes have been identified and discussed; unfortunately such a study could not raise the interest or awareness of the management and was not given the green light. Nevertheless, early discussions confirmed the requirements formerly identified in other types of batch processes; these constraints are reviewed at the beginning of *Chapter 2*.

## 1.2 Comparison with Combinatorial Methods

Combinatorial methods based on simplifying assumptions have been proposed by others authors. They feature the inherent advantage of automatically providing the designer with reasonably good heat integration solutions in a fraction of the time needed to manually design HENs using a Pinch Analysis approach. The comparison focuses on the performance of the different methods in terms of heat recovery and costs (not of required time) in order to assess the respective potentials of the methods. For more details, please refer to the report by Krummenacher & Auguste, 1997.

### 1.2.1 Design of Direct Batch HEN with the Omnium Verfahren

The Omnium Verfahren (OV) (Hellwig & Thöne, 1994) is a simplified combinatorial method based on the assumption of exclusive hot stream-cold stream matches. It searches for the combination of exclusive matches featuring the highest heat recovery, which is stated as an allocation problem and solved by a modified Hungarian Algorithm.

For the comparison, the Pinch Analysis (PA) based design methodology is restricted to direct heat exchanges. Solutions obtained with the PA feature higher heat recovery and least total annual costs. PA HENs include a larger number of process-to-process heat exchangers (HEXs), while the OV HENs require more utility HEXs. The assumption of exclusive matches to reach economic optimum does not hold in general, but allows for the automatic HEN design Comparisons achieved by other authors confirm these results (Uhlenbruck, 1995; Uhlenbruck &Vogel, 1999).

### 1.2.2 Design of Indirect Batch HEN with the Permutation Method

The Permutation Method (PM) (Stoltze *et al*, 1992, 1995) assumes that all heat exchanges are achieved through intermediate heat storage (irrespective of the time schedule of streams). Based on simplified stream-storages matching rules, an exhaustive search of the most cost-effective set of stream-storages matches is performed.

In this case, the PA approch is based on the TAM (time average model) composites (Kemp & Deakin, 1989) and on simple rules for the assignment of heat storages. The heat recovery schemes designed by the PA a more cost-effective, and feature a higher heat recovery (at least in the case of pinched processes). The PA schemes benefit from the available temperature driving forces, while the PM neglects this opportunity (e.g. when mixing between heat storage units (HSUs)).

The PA features the advantage of providing insight in and understanding of the major issues (e.g. selection of storages), while the automated PM allows to easily design good HENs. The extend to which the PA designs outperform the PM ones depends of course on the particular process features (important combinatorial effects), but also on the assumed cost functions for heat exchangers (HEXs) and heat storage units (HSUs). Reasonable cost models (i.e. cost functions with small fixed cost parameters) are generally favorable to the PA designs.

## 1.3 Batch Process Issues: Simplication, HEX Re-use, Rescheduling

Batch processes feature numerous particularities. If some essential practical constraints are not taken into account, the proposed solutions may turn out to be infeasible; while taking every process data for granted (e.g. the actual schedule) will likely lead to impracticable problems or overlook major opportunities. Guidelines for data extraction and a suitable format to specify batch process data relevant to heat integration are proposed.

### 1.3.1 Preliminary Process Simplification

Actual industrial processes usually features a large number of time slices. If schedule specifications were taken as such, the analysis and/or design would at worst be impraticable, at best uneconomic and highly sensitive to schedule variations. Guidelines are proposed for the preliminary analysis and simplification stage (refer to *Section 3.4* on page 106):

1. eliminate "artificial", meaningless time slices generated by streams not relevant to the process-to-process heat integration, or by soft streams which schedule can be modified;
2. identify parts of streams responsible for small / highly schedule sensitive time slices and remove these parts from the heat integration;
3. neglect streams of small duration and/or small heat content.

A simple criteria is proposed, which takes the relative benefit associated with a stream heat contribution into account. This criteria allows to apply guidelines 2) and 3) in a systematic manner.

### 1.3.2 Constraints Limiting the Re-use of HEX Units

Like other batch equipments, HEX units can be re-used accross time slices to decrease capital costs. Repipe and/or resequence of HEXs have been proposed by other authors, but the actual conditions which make these modes of re-use feasible were not.

Different constraints limiting the repipe opportunities are identified and classified in 3 categories:

1. the compatibility of thermo-physical properties of the streams (with respect to the type of heat exchanger to be used);
2. the chemical compatibility of the streams (and the feasibility of cleaning at affordable costs);
3. operational constraints resulting from the time schedule of the streams.

Constraints 1. and 3. also restrict the resequence opportunities.

The consideration of constraints of the first category allows to form groups of streams. Within each of these groups, the consideration of constraints 2) and 3) in a matrix format further restricts the feasible repipes (refer to *Section 3.2* on page 76).

### 1.3.3 Rescheduling

The required capacity of HSUs depends on the relative phase difference between heat supply to, and heat removal from a storage sub-system, hence on the schedule of streams. To assess opportunities for a capital costs decrease, the potential effect of rescheduling a stream is easily identified when the cumulated heat contribution of that particular stream is represented against the "background cumulated heat contribution" of the other streams (refer to *Section 2.5* on page 66). On this graphical representation, various rescheduling alternatives (delay, advance, change of flowrate - whenever feasible) are readily compared.

# 1.4 Design of Indirect Heat Recovery Schemes

## 1.4.1 Heuristic Pinch Analysis Based Method

The PA inspired design of indirect HR schemes used to compare with the PM method has been further developed into a systematic method. The amount of HR is chosen as the basic independent variable, while the number of HSUs is another key structural variable. For any given feasible HR (i.e. process $\Delta T_{min} \geq 0$), the corresponding minimum number of HSUs can be determined from the TAM (energy) composites, the supply temperature and schedule of the streams. The advantages and drawbacks of considering slice-wise instead of stream-wise supply temperatures is also analysed.

The basic rules to identify the need for intermediate HSUs are not new, but the construction of the so-called "limiting supply temperature profiles" (LSTPs) on the TAM composites allows to formalize these rules and identify the HR and temperature assignment ranges of each HSU. It provides additionally a graphical insight in the problem (e.g. to identify usefull process changes with respect to the number of HSUs). The procedure assumes vertical heat transfer between TAM composites, which is a valid first order approximation (refer to *Section 2.2* on page 19).

The systematic design method makes use of heuristics rules derived from experience. The integer decisions (number of HSUs, assignment of HSUs to streams, which stream has to be integrated within each storage sub-system) as well as the operating temperature of HSUs can be optimized, while detailed optimization (fine tuning of the heat contribution to each storage sub-system) cannot be efficiently addressed.

The method (refer to *Sub-section 2.3.2* on page 47) first assumes vertical heat transfer between TAM composites, and for a given number of HSUs, systematically evaluates the total annual costs (TACs) while the heat recovery is increased. An upper limit to the heat recovery appears when the operating temperature of one or several HSUs is fully "pinched". Each time a bottleneck appears, the cause is identified and alternate solutions to remove it are systematically searched for (e.g. by changing the assignment of HSUs, increasing the HR beyond the upper vertical limit by removing constraining streams or resorting to criss-cross heat exchanges around a HSU). The preliminary screening assuming vertical heat transfer and different number of HSUs helps to focus later on most promising HR ranges.

In indirect heat recovery, the storage pinch plays an key role, and most often limits the heat recovery before the process pinch comes into play. But unlike process $\Delta T_{min}$, optimum storage $\Delta T_{min}$ as low 1-2 °C are commonly found. This surprising result is explained by considering the actual temperature driving forces. When implemented in an Excel Worksheet, the operating temperatures of HSUs are efficiently optimized using the Excel Solver (although this optimization has often a second order effect).

Guidelines to identify direct heat exchange matches which would likely improve the cost-effectiveness of the heat recovery without making it sensitive to schedule variations are derived (refer to *Section 2.4* on page 63). This allows for a simplified, but robust, mixed direct-indirect heat recovery to be achieved, to the expense of additional degrees of freedom and related optimization difficulties.

### 1.4.2 Mathematical Model and Genetic Algorithm Based Optimization

A simple mathematical model for the synthesis of indirect HR schemes is presented (*Sub-section 2.3.1* on page 40), and a genetic algorithm (GA) based solution approach is proposed to solve the synthesis problem (refer to *Sub-section 2.3.3* on page 58) The approach includes two levels:

- at the upper level, the operating temperature of each HSU is optimized. These temperatures determine the structure of the feasible HENs;
- at the lower level, the structure of the HEN is fixed, and the heat rate (or alternatively the output temperature) of each HEX is optimized.

In this approach, the number of HSUs is defined externally by the user (i.e. the GA optimization should be performed for several numbers of HSUs). A dimensionless coding of the independent variables to be manipulated by the GA should prevent the genetic operators to produce "infeasible" individuals (i.e. which do not satisfy the constraints), and hence likely increase the efficiency of the search.

## 1.5 Design and Optimization of Direct Batch HEN

A GA based strategy is proposed for the synthesis of direct batch HENs (refer to *Section 3.3* on page 88). The strategy features a decomposition into two levels:

- at the upper level, master HENs (i.e. masterstructures and the related HEX area values) are postulated (randomly generated) and optimized using a GA (on the basis of the fitness factor provided by the lower level);
- at the lower level, a masterstructure is particularized to each time slice of the cycle period, taking the HEX re-use opportunities (feasible repipe/ resequence opportunities) into account, leading to one or several so-called slice-wise structures. For each slice-wise structure, the heat recovery is optimized (maximized), subject to the constraints of the maximum area values specified at the upper level. The consistent sequence (i.e. obtained by feasible structural modifications from a time slice to the next) of slice-wise structures featuring the highest heat recovery (lowest total costs) is identified and feed to the upper level as a measure of the fitness of related master HEN.

As a result, the AG approach will not provide a single, but a population of good master HENs, from which it is possible to chose, according to additional criterias not accounted for during the optimization.

The proposed approach uses a simple coding of the masterstructure (proposed by other authors for continuous HENs). The no-stream-split assumption is reasonable in the context of batch HENs, which are already complex enough as a result of structural modifications associated to repipes or resequences. The complexity of the HENs is further controlled by the number of HEX units to be included in the master HENs.

The lower level problem of maximizing the heat recovery of a slice-wise HEN, subject to the constraints of maximum area values, is obviously a NLP problem, for which a suitable solution approach - deterministic solver or stochastic algorithm - remains to be chosen.

## 1.6
## PinchLENI & LENIpass

Unlike initial expectations, only minor new features have been implemented in the PinchLENI software: the batch cascade curves (BCC) are now time slice related, the pinch temperature graph highlights the temperature range of heat source and heat sink of each time slice, and the data structure for batch processes has been modified to avoid memory management problems observed during supertargeting. Major bottlenecks to further implementation work have arisen, due to both the data structure and the internal organisation and management (refer to Krummenacher & Auguste, 1997).

Funding external to the PinchBATCH project has initiated the re-programmation of the presently called LENIpass software in the Java language. The implementation rate has been significantly lower than expected, hindered by the high update rate and quick evolution of the Java language and environment (some features of which are essential to the LENIpass implementation), by the underestimated preliminary phase of software specification, by the intrinsic difficulty of simultaneously developing methods and planning their implementation, and finally by the early leave of the Java programmer.

The LENIpass software is designed to include 3 main modules - LENIpfd, LENItarget, and LENIdesign - reflecting three important activities in process integration which are the process definition and documentation, the analysis and screening of heat integration opportunities (targeting), and the actual design of HENs. The state of implementation is as follows (refer to *Appendix B*):

- LENIpfd implements the basic features of a flowsheeting software tool, while all other features (e.g. equipment and task definition, scheduling) have only been specified in details but are not yet implemented;
- in LENItarget, basic PA tools (composites, grand composite) have been implemented, while a stream editor is in development. In the perspective of a software suitable to end-users, facilities such as user-selectable input and output units and formats, general graph formats including cursors measurements, specification of relative position of composites curves by mean of the amount of high or low utility, as an alternative to $\Delta T_{min}$, are also available. Targeting tools and algorithms remain to be implemented;

- for LENIdesign, only preliminary draft specifications are available at this stage.

A large potential is now available under the form of detailed specifications, which have required a significant amount of work to devise. Particular attention has been paid to:

- the general organization and the graphical user interface (self-explained and uniform GUI, intuitive data/file handling well suited to Pinch Analysis projects, a contextual help, etc.);
- a systematic definition of the available equipments, their assignment to various processes, the task definition of each process, the specification of stream data, various alternative short-term production planning (macro-scheduling), definition of period of analysis and representation on Gantt diagrams. The procedure benefits from its accordance with the batch engineering practice, and LENIpfd shall provide the end-user with the necessary tools to address the close links between process equipments, their scheduling, time-related constraints, and heat integration opportunities;
- the way various user-defined targeting routes can be specified and saved in LENItarget. The definition of utilities, HEXs, HSUs and their related economic parameters, the definition of the objective function are also addressed;
- improvements to the HEN graphic editor of PinchLENI as revealed by experience (e.g. the lack of mixers, by-pass and valves; misleading representation of streams which do not cross the pinch; the opportunity to impose the area of a match, not only its heat rate or temperature; the misleading indication of a mean $c_p$ for multi-segment streams; the difficult multiple pinch design; the fact that cross-pinch HEXs are not allowed - but needed in MBC/batch HEX design; the impossibility to delete HEXs while other HEXs exist "downwards away from the pinch", etc.). A general HEX model has been developed and implemented as an independent Java module (Java Bean); the model can solve the remaining HEX design and operating variables from any consistent set of specified variables.

## 1.7 Perspectives for Further Work

The PinchBATCH project had to address various issues (e.g. practice related constraints, process simplification) before developing methodologies for the design of batch HENs. Several approaches arising from PinchBATCH require further work. The very next steps should be concerned with:

- the implementation and the validation of the proposed GA based design and optimization approach for indirect batch HR schemes. The validation requires the application on at least 5-10 processes, and sensitivity studies to several parameters to make sure the provided solutions are consistent with expected results;
- the implementation and the validation of the GA based design and optimization approach for direct batch HENs. A thorough validation procedure (similar to that for the indirect HR schemes) is essential;
- the implementation of the proposed simplified PA based heuristic method for indirect HR schemes. Optimum HR schemes obtained using the GA approach shall serve as reference;
- the possible extension of the GA based optimization to mixed direct-indirect HR schemes;
- the demonstration, on the basis of 2 industrial batch processes, of the overall procedure resulting from the application of the various tools provided for the preliminary process analysis and simplification, the targeting of the HR modes, the design and optimization, and consideration of rescheduling opportunities, schedule variations, etc.

The following tasks are to be considered in second priority:

- the detailled consideration of schedule variation issues and possible ways to account for these variations at the targeting and design stages;
- the development of simplified targeting methods for indirect and mixed direct-indirect HR schemes. The validation of these methods shall benefit from reference solutions obtained using the GA based optimization;
- the consideration of hot process water needs at the targeting stage (the GA based optimization should account for this issue at the design stage);
- and finally the implementation into the LENIpass software. The tools and methods for the heat integration of batch processes obviously require to

be implemented in a software package to make these suitable for practice. Experience has shown that the associated work should not be underestimated. A development team is necessary, and this task should preferably be assigned to a company specialized in process simulation.

# Chapter 2

# INDIRECT HEAT RECOVERY

## 2.1 Introduction

### 2.1.1 Motivation

Indirect heat recovery (HR) has generally been disregarded, as being *a priori* a costly mean of heat integration, although costing procedures or cost targets have seldom been proposed for heat storage so as to justify this assertion ! Therefore, heat storage has only been considered as a possible complement - after opportunities of direct heat recovery have been exhausted - rather than a full heat integration mode. Rescheduling has often been advocated to increase the direct heat recovery potential so as to avoid resorting to heat storage.

The direct heat integration of batch processes using the time slice model implicitely assumes a stiff scheduling of the streams. Experience with various batch processes has shown that this is in most cases too crude an assumption. Both systematic and stochastic variations of the schedule are common due to:

- the fouling of heat exchangers and reactors, leading to heating/cooling tasks of increasing duration, and requiring regular disruption of the batch cycle time for cleaning;
- feeds or products of varying specifications, requiring adaptations of the recipe (temperature, duration, etc.);

- the use of qualitative or quantitative parameters as a criteria to terminate a task, i.e. a task is not primarily defined by a fixed duration, but rather continues until the controlled parameter reaches the specified target value;
- a poor automation of many batch plants, making the actual schedule dependent on the operators;
- possible failures of equipments, leading to unexpected delays and requiring the use of alternate processing routes.

Detrimental effects on the product quality or energy savings arising from accidental schedule variations could be tolerated, while penalties due to systematic variations are not acceptable.

Flexibility and operability are highly desired features of batch plants. Energy savings are not given a high priority level, while production capacity and quality are often considered as key objectives. Heat recovery schemes which constrain these objectives would be disregarded in practice.

The rescheduling of certified processes to improve opportunities for direct heat integration is often not possible or economically not justified, since the certification procedure (developed internally or externally to the company) is lengthy and costly. Other constraints which rule out or mitigate the use of the direct heat recovery mode include:

- critical processing steps (e.g. reactions, etc.) cannot be integrated with other process streams for safety or quality reasons;
- batch processing is used for many speciality chemicals, characterized by a short economic lifetime and a related striving after the shortest time to market as possible. Production generally starts while several process parameters (in particular the schedule) are not well defined yet and are likely to evolve as a result from experience;
- solid streams or high viscosity liquids heated/cooled in jacketed reactor, generally require the use of an intermediate heat transfer fluid;
- complicated actual time schedule: stream tables of batch processes often result from severe simplifications with respect to time, while their actual schedule might well require the definition of additional time slices and invalidate part of a direct heat recovery network previously developed on the basis of a simplified stream table.

Aware of the fact that the schedule and the resulting decomposition into time slices are subject to variations, two main approaches - progressing somewhat in opposite directions - can be considered:

1. develop/optimize direct heat recovery schemes for the base case schedule, then analyse the sensitivity of these schemes to the most likely variations of schedule, and resort to indirect heat recovery for problematic matches, if need be;
2. in order to remove the stiff timing constraint, start by developing 100% indirect heat recovery schemes, then remove from these schemes and integrate in direct mode only those matches which are not sensitive to schedule variations («robust direct matches»).

With respect to the first approach, the various causes of schedule variations are generally non-correlated, so that numerous cases should be considered, making this approach difficult and costly. For this approach, methods for modeling the delays and their propagation / compensation throughout the schedule of a batch remain to be developed to a large extend, although this aspect has already been considered in the EUROBATCH Project (Klemes *et al.*, 1994). Not every delay will result in a new time slice or in an infeasibility of the heat recovery network. In addition, the decomposition into time slices has been experienced as difficult to manage when adressing the trade-off direct <-> indirect heat recovery, due to the lack of a global overview.

In view of these difficulties, and given the advantages of flexibility and low sensitivity to scheduling variations, the second approach has been prefered in the course of this project and forms the core of this chapter. In this perspective, direct heat exchanges are more an exception than the rule. But the design of robust direct heat recovery schemes would be an important objective of future research (refer to Chapter 4 on page 119).

Designing 100% indirect heat recovery is actually not a new proposal; Stoltze *et al.* (1992, 1995) have already addressed this issue using the so-called Permutation Method (PM), later improved by Mikkelsen (1998) (refer to *Sub-section A.3.2* on page A-9 for a detailled review). But the first part of this project (Krummenacher & Auguste, 1997) has demonstrated potential benefits from using a Pinch Analysis based approach, which also has the advantage of providing more insight in the problem, while the Permutation Method is rather a black box approach.

### 2.1.2 Main Issues

In indirect heat recovery systems, heat from hot streams is first transfered to storage streams, which are stored, until it is finally transfered to cold streams when needed. Designing indirect heat recovery schemes is all about inserting some kind of "storage composite" between the hot composite and the cold composite. So, what is so difficult in designing such systems, what are the independent variables available to the designer, and what are the major trade-off effects ?

The example process EP1 (formerly called Ex1), which has already been presented and analyzed in Krummenacher & Favrat (1995) and in Phase 1 (Krummenacher & Auguste, 1997), is used as an illustration throughout this chapter. The Time Event Model (Gantt diagram) of this process is depicted

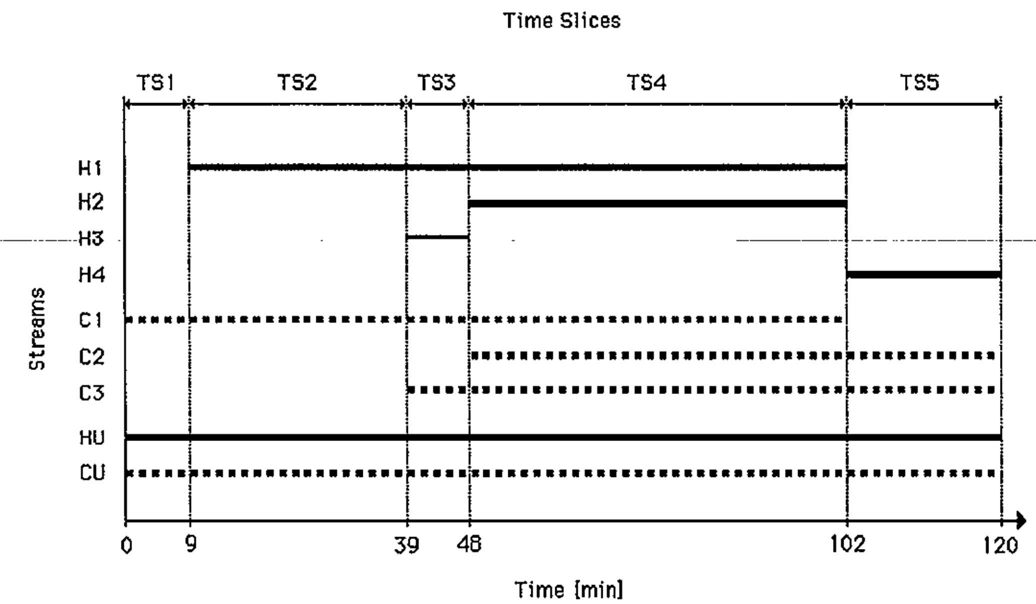


**Figure 2-1** Time Event Model of the EP1 example process.

on *Figure 2-1*, while stream data are summarized in *Table 2-1*.

*Figure 2-2* represents the TAM composites (in energy) for process $\Delta T_{min}$=11.5°C, and one possible "storage composite". The proposed storage system includes 4 heat storage units (HSUs) which are assumed to be of the constant temperature / variable mass (FTVM) type [1]. The temperature margin (or temperature window) of each HSU, defined as the possible range

| Stream Name | T in [°C] | T out [°C] | MCp [kW/°C] | Heat Rate [kW] | Heat [kWh/bat.] | t start [min] | t stop [min] | h [W/m2°C] |
|---|---|---|---|---|---|---|---|---|
| C1 | 25 | 100 | 1 | 75 | 127.5 | 0 | 102 | 1000 |
| C2 | 130 | 180 | 3 | 150 | 180 | 48 | 120 | 1000 |
| C3 | 80 | 105 | 5 | 125 | 168.75 | 39 | 120 | 1000 |
| H1 | 135 | 15 | 1.1 | -132 | -204.6 | 9 | 102 | 1000 |
| H2 | 100 | 95 | 20 | -100 | -90 | 48 | 102 | 1000 |
| H3 | 165 | 125 | 3.5 | -140 | -21 | 39 | 48 | 1000 |
| H4 | 165 | 125 | 3.5 | -140 | -42 | 102 | 120 | 1000 |
| HU | 191 | 190 | Util | | | 0 | 120 | 1000 |
| CU | 10 | 11 | Util | | | 0 | 120 | 1000 |

**Table 2-1** Stream table of the EP1 example process.

of operating temperature for that HSU, is determined using rules that have been independently proposed by Krummenacher & Favrat (1995), and Sadr-Kazemi & Polley (1996) (refer to *Sub-section A.2.2* on page A-4). Since an additional intermediate HSU has to be introduced whenever the temperature margin of an existing HSU falls to 0°C or below, these rules also allow to target for the minimum number of HSUs. These rules and their systematic formulation are described in *Section 2.2* on page 23.

As depicted, the global heat recovery system includes 3 storage sub-systems, namely Sss1-2, Sss2-3, Sss3-4. Each sub-system operates in a vertically defined heat recovery region, e.g. the sub-system Sss3-4 recovers heat from the hot composite from 165 downto 100°C, and supplies heat to the cold composite from 88.5 up to 103.8°C. Links between sub-systems exist since, e.g., HSU3 is the hot storage of the sub-system Sss2-3, and at the same time the cold storage of the sub-system Sss3-4.

But TAM composites are neither representative for the heat rate of the streams, nor for the required heat transfer area. In addition, the heat transfer film coefficients of the streams are often quite different. It is well known from continuous processes that the assumption of vertical heat transfer from hot to cold composites leads to inaccurate targets when the film coefficient are

1. FTVM storage is assumed because of its wide applicability. Stratified heat storage units, commonly used in HVAC as buffer tank, have been proposed by Krummenacher & Favrat (1995) for heat integration application. Although heat storage systems based on stratified heat storage are cheaper and simpler to design and optimize, they lack flexibility in practice and suffer from heat degradation problem at the interface between the cold phase and the hot phase.

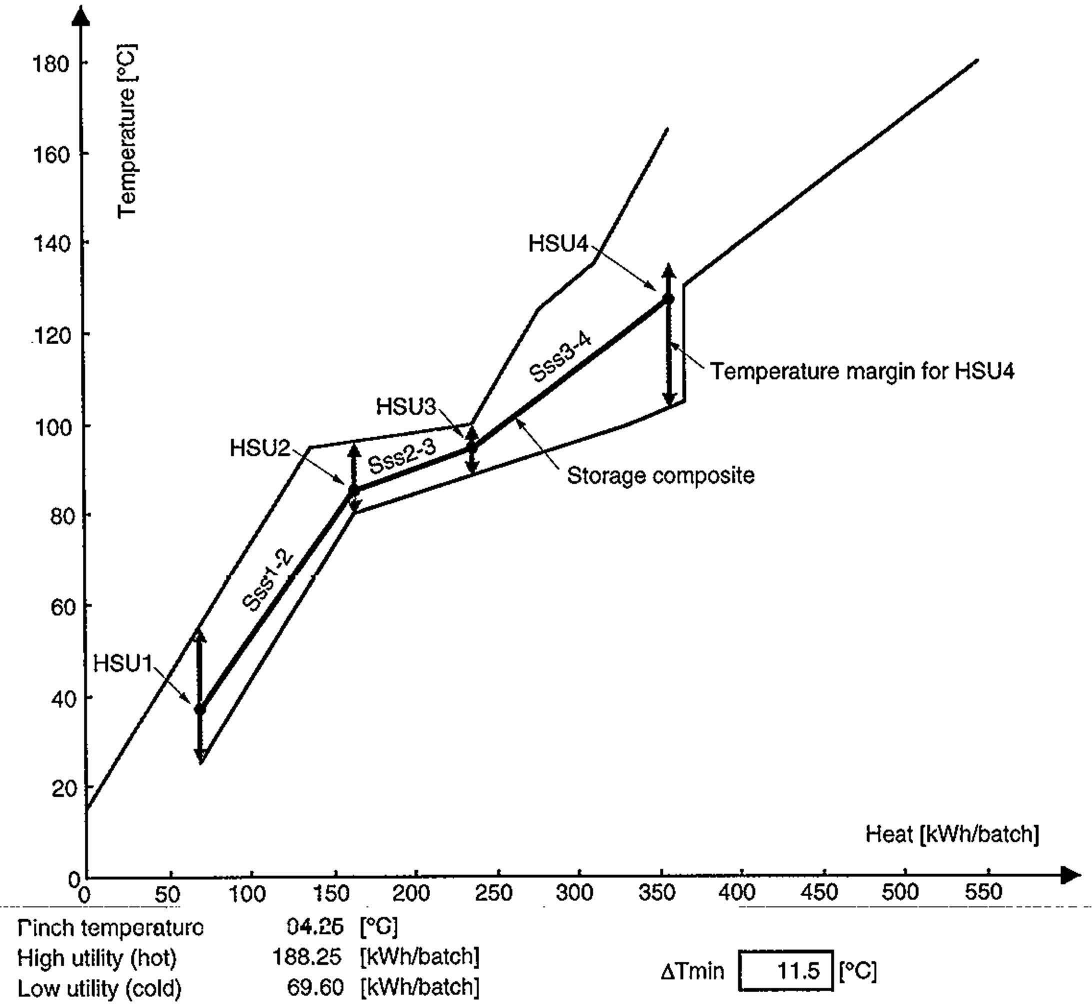


**Figure 2-2** TAM (energy) composites, heat storage units, and storage composite (batch example process EP1).

significantly different (e.g. in a ratio larger than 1 to 10) (e.g. refer to Townsend, 1989), while the actual minimum would include significant criss-cross heat exchanges. This observation certainly holds for TAM composites too, i.e. the assumption of "vertical" partition of TAM composites into storage sub-systems might lead to solutions that significantly deviate from the optimum one.

The designer is ultimately interested in identifying the most cost-effective heat recovery scheme, requiring that major degrees of freedom (DOFs) be explored and optimized (costs are made up of energy costs, annualized heat exchanger costs and annualized storage costs). These include (assuming a 100% indirect heat recovery):

1. the amount of heat recovery (or $\Delta T_{min}$, by analogy to the single DOF of continuous processes at the targeting stage);
2. the number of HSUs, which is a fundamental structural dimension of the problem. The optimal number of HSUs might well be larger than the minimum number of HSUs for the same level of heat recovery;
3. the actual assignement of the HSUs, i.e. which heat recovery region is assigned to (or "covered by") each storage sub-system;
4. the operating temperature of each of the HSUs, which has to be optimized, because of the global trade-off between storage costs and heat exchangers costs;
5. the "cut-off" temperatures of each stream with respect to the storage sub-systems (i.e. the heat contribution of each stream to each storage sub-system), subject to the constraint of heat balance of each sub-system. As mentionned earlier, for targeting purposes, the vertical partition of composites to define the storage sub-systems might well be acceptable. But a detailled optimization of designs requests that this simplifying assumption be removed. This will account for variations of heat transfer film coefficient and "duty ratio" of streams, but also for the effect of the sequence of sink/source of heat on the storage volume and of the constraining supply temperatures. Note that the requirement for heat balance of each sub-system could be relaxed, leading to design conditions similar to the PM proposed by Mikkelsen (1998), reviewed in *Sub-section A.3.2* on page A-9.
6. the rescheduling of streams (in particular storable process streams) to decrease the size of costly HSUs, if rescheduling is acceptable (indirect heat recovery is less sensitive to scheduling variation than direct heat recovery, but still the capacity of HSUs can be influenced);
7. the possible re-use of HEXs between streams which exhibit similar thermo-physical properties and which are chemically compatible.

Despite these numerous DOFs, indirect heat recovery networks are structurally much simpler compared to direct HENs, in that there is no need for splitting process streams since the flowrate of storage streams can be freely adjusted.

Note also that if direct heat integration of some beneficial matches has to be simultaneously optimized, additional DOFs are introduced (e.g. the $\Delta T_{min}$ of each match), while the overall HR is specified.

The complexity of optimization is also increased whenever hot process water streams are present, since such streams could be directly extracted from water-based storage systems (use mixing as required to provide the desired target temperature), instead of heating them indirectly by storage streams (requiring additional heat exchangers units and area).

The use of water as a storage medium is limited to temperatures below 100-120°C; above this limit, other storage fluids (e.g. thermal oil) or other types of heat integration (e.g. through utility network - low pressure steam) should be applied.

### 2.1.3 Organization of the Chapter

This chapter is a central part of the report and includes all developments related to indirect heat recovery and heat storage.

The next section (*Section 2.2* on page 23) builds on rules proposed by Krummenacher & Favrat (1995), and Sadr-Kazemi & Polley (1996) and presents a methodology to determine the minimum number of HSUs and the available margin for assigning the HSUs, given a HR level. Explained on the basis of a graphical representation which provides insight in the problem, the methodology may also be implemented in a computer programme. The important concept of storage pinch is explained. The similarities and differences of the time slice related supply temperatures (Krummenacher & Favrat, 1995) and the stream related supply temperatures (Sadr-Kazemi & Polley, 1996) are highlighted.

*Section 2.3* on page 44 addresses the search for minimum costs, 100% indirect HR schemes. The corresponding mathematical model is presented first, followed by the description of a heuristic procedure based on Pinch Analysis (*Sub-section 2.3.2* on page 51). An automated synthesis approach based on Genetic Algorithms (GAs) is also developed in *Sub-section 2.3.3* on page 62.

The case of mixed indirect & direct heat recovery is considered in *Section 2.4* on page 67. Guidelines to identify promising matches for direct HR and the choice of independant optimization variables are described. The procedure is explained on the basis of the process EP1 and results are compared to both the 100% indirect and 100% direct heat recovery.

*Section 2.5* on page 70 demonstrates how opportunities for decreasing the capacity (hence the capital costs) of HSUs through rescheduling of individual streams can be assessed using a simple graphical representation.

Finally, *Section 2.6* on page 73 summarizes the content of this chapter.

## 2.2 Selecting Heat Storage Units

### 2.2.1 Overview

The overall level of HR (e.g. in [kWh/batch]) is specified, part of it through direct heat exchanges, the remaining through indirect heat recovery using heat storage.

Given the corresponding energy composites (refer to *Figure 2-2* on page 20), how many heat storage units (HSUs) are required, i.e.what is the absolute minimum number ? There is of course no single answer to this question, since it depends on the type of HSUs to be used. But in any case, the number of HSUs strongly influences the whole structure of heat recovery network and its complex trade-off effects, and hence the profitability.

Kemp & Deakin (1989) assumed constant temperature HSUs. Given a minimum temperature approach (MTA or $\Delta T_{min}$) with both hot and cold process streams, the stage-wise heat storage composite is easily calculated . The number of stages (temperature levels) defines the required number of HSUs. Constant temperature storage can be realized in practice by latent heat storage (phase change material, including steam accumulator). Although featuring high specific heat capacity, latent heat storage materials are generally expensive, may be unstable in the long term, and are not necessarily available for the required temperature level. But constant heat storage may be the right solution for heat recovery between pinched, horizontal energy composites, for which sensible heat storage would require large capacities.

Krummenacher & Favrat (1995) considered stratified HSUs for heat recovery from batch cascade curves. They observed that the "supply" temperatures of both hot and cold contributions of time slices constrain the temperature of HSUs and proposed rules for placing intermediate HSUs.

Sadr-Kazemi & Polley (1996) (refer to *Sub-section A.2.2* on page A-4) made the same observation on energy composites (assuming 100% indirect heat recovery). They proposed rules similar to those of Krummenacher & Favrat (1995), but related to the individual streams (instead of time slices).

In practice, several types of HSUs may be required for the heat integration of a single process: constant temperature/variable mass heat storage for steep parts of energy composites, constant temperature heat storage (phase change material) for horizontal parts of composites (if heat integration through the utility steam system is not possible).

Rules to identify the need for intermediate HSUs have been suggested, but their formalization into a systematic procedure suitable for computer implementation has not. A representation allowing for a better insight in the problem and the possible trade-offs is also required.

## 2.2.2 The Storage Pinch

Before describing the proposed method for the definition of the minimum number of HSUs, the concept of storage pinch ($\Delta T_{minSto}$) has to be introduced. The storage pinch $\Delta T_{minSto}$ is basically a temperature pinch, like the well-known process pinch ($\Delta T_{minPro}$), in that heat can only be transfered from a hot process stream to a storage stream (or from a storage stream to a cold process stream) if a positive temperature driving force exists.

Compared to the process pinch, a storage pinch features the distinctive property of not being apparent on the energy composites (extended to include the "storage composite"). Storage pinches are at the root of the definition of the minimum number of HSUs, and result from the desire to keep the number of HSUs as low as possible, for both operability and economic reasons.

*Figure 2-3* highlights a storage pinch with cold streams and the way the actual temperature driving forces can be represented. This case is part of the cost optimal solution to a mixed direct-indirect heat integration of the example process EP1. The operating temperatures of HSUs (HSU2: 99.001°C, HSU3: 130.6°C}, as well as their temperature margin (HSU2:1°C; HSU3: 5°C) are imposed by adjacent storage sub-systems (refer to *Section 2.4* on page 67).

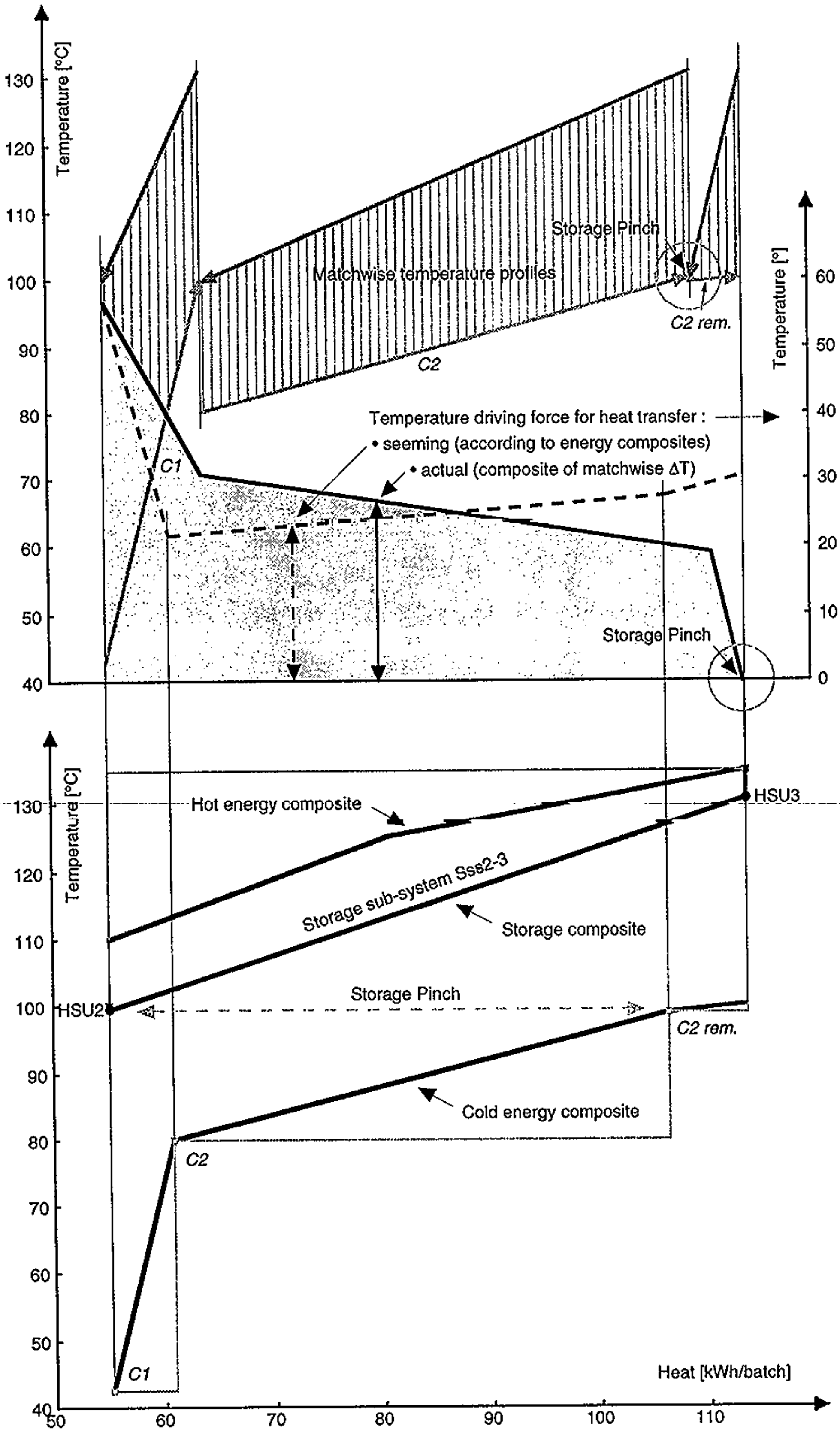


**Figure 2-3** Storage pinch and related temperature driving forces representation (refer to comments in the text).

The lower part of *Figure 2-3* represents a portion of the (energy) composites, to be heat integrated through the heat storage sub-system Sss2-3. The cold composite includes three streams (C1, C2 and C2 rem., defining the cold «limiting supply temperature profile» - a concept presented in *Sub-section 2.2.3*), while the streams actually included in the hot composite do not matter for the discussion here. The lowest temperature of storage HSU2 is imposed by the supply temperature of C2 rem. The temperature driving forces (TDF) when transfering heat from Sss2-3 to C2 rem., tends towards zero; in other words a storage pinch appears.

The upper diagram decomposes the storage and cold composites to represent the match-wise temperature profiles between the splitted stream associated to Sss2-3 and C1, C2 and C2 rem., respectively. The storage pinch ($\Delta T_{minSto}$=0) is present at the cold end of the match «Sss2-3»-C2 rem. Test cases indicate that economical storage pinches can be in the order of 1°C or even less, which are quite seldom found in continuous processes. These surprising small $\Delta T_{minSto}$ values actually result from the fact that they are related to a very local effect, i.e. pinched heat transfer applies only to a small amount of heat. They are also found because of complicated direct-indirect heat integration effects.

The matchwise temperature profiles can be «composed together» by sorting them in decreasing order of magnitude so as to represent the actual TDF from Sss2-3 to the cold streams; the storage pinch and its very local effect is clearly identified on the right. The dotted line represents the seeming TDF, as derived from the energy composites represented on the lower diagram. Note that it does not matter whether the matchwise temperature profiles are «composed» in increasing or decreasing order of magnitude. In order to assess the actual effect of the storage pinch in term of heat transfer area and related investment costs, one should weight the match-wise temperature profiles by the relative duration of the related streams.

If the storage composite included as many HSUs as the number of process streams, i.e. where a HSU is assigned to each supply temperature of either the hot or the cold energy composites, there won't be any storage pinch effect and the actual TDF would be equal to the TDF available between the energy composites and the storage composite (i.e. the heat would actually be transferred vertically from the hot composite to the storage composite, and then from the storage composite to the cold composite). The limitation to heat recovery would arise from the process pinch itself.

But a design featuring a large number of rather small HSUs (i.e. a number of HSUs significantly in excess of the minimum number of HSUs) would not be economical: not only are HSUs of small capacity a poor design (from an energy and economics point of view), but they would require a large number of small HEXs too. As opposed to continuous processes, it appears that for most batch processes (depending on both the schedule and the discrepancy of the supply temperatures of the streams), the process pinch has a small effect on the optimal heat recovery, while the storage pinches (hence the number of HSUs) are deciding the optimal trade-off between heat recovery and capital costs (before any process pinch comes into play).

### 2.2.3 Defining the Minimum Number of Heat Storages

Consider e.g. the energy composites represented by *Figure 2-2* on page 20. Searched for is the minimum number of storage units, assuming:

- ♦ constant temperature/variable mass heat storage units;
- ♦ a minimum temperature approach ($MTA_{Sto}$ or $\Delta Tmin_{Sto}$) specified between process streams and storage streams. To simplify, it is first assumed that $\Delta Tmin_{Sto}=0$ as a limiting case, then $\Delta Tmin_{Sto}>0$ will be considered (but recall that unlike process pinch, storage pinch can, in some instances, be very small indeed);
- ♦ the heat recovery range of storage sub-systems from hot process streams to cold process streams are vertically aligned.

Before describing the procedure for determining the minimum number of intermediate HSUs, let's make some points clear:

- ♦ to totally recover heat from the vertically defined heat recovery regions, first and last storage units have to be located at the cold end and the hot end of the region, respectively. The problem is actually the number and the location (temperatures, heat recovery range) of intermediate HSUs;
- ♦ the rule proposed by Sadr-Kazemi & Polley (1996) (refer to *Sub-section A.2.2* on page A-4) can be formulated as follows: the operating temperature of any HSU has to higher than the highest supply temperature of cold streams included in the storage sub-system on the right (for which the considered storage is the «cold» storage of the sub-system), while it also has to be lower than the lowest supply temperature of hot streams included in the storage sub-system on the left (for which the considered storage is the «hot» storage of the sub-system). Hence the operating

temperature of a storage is constrained upwards by hot streams, while it is constrained downwards by cold streams. The proposed systematic procedure is an application of this formulation;

- the above formulation actually contains several cases: an intermediate storage can be imposed (i.e. the heat recovery range of the storage sub-system be limited) by cold streams only, by hot streams only or by both;
- to minimize the number of HSUs, the heat recovery range (or region) of a heat storage sub-system has obviously to be maximized. The starting point can be either the hot end or the cold end of the heat recovery region, providing two limiting cases (see below).

### 2.2.3.1 *Limiting Supply Temperature Profiles*

Given the TAM (energy) composites, first draw the «limiting supply temperature profiles» (LSTPs), some kind of «staircase temperature profiles» which defines the actually most constraining cold (hot) stream supply temperature as a function of the vertically corresponding position on the cold (hot) composite.

The cold LSTP is drawn according to the following rules (refer to *Figure 2-4*):

- start at the lowest supply temperature and move horizontally to the right, until a new supply temperature is vertically crossed;
- at this point, move vertically to this temperature on the cold composite;
- again, move horizontally until the next vertically aligned supply temperature;
- continue until the last supply temperature;
- move vertically to the hot end of the cold composite when vertically aligned with this point.

In this way, the cold staircase profile begins at the cold end of the cold composite and ends up at the hot end of the same composite.

The hot LSTP is drawn in a similar manner, except that it starts from the hot end of hot composite and proceeds to the left towards the cold end.

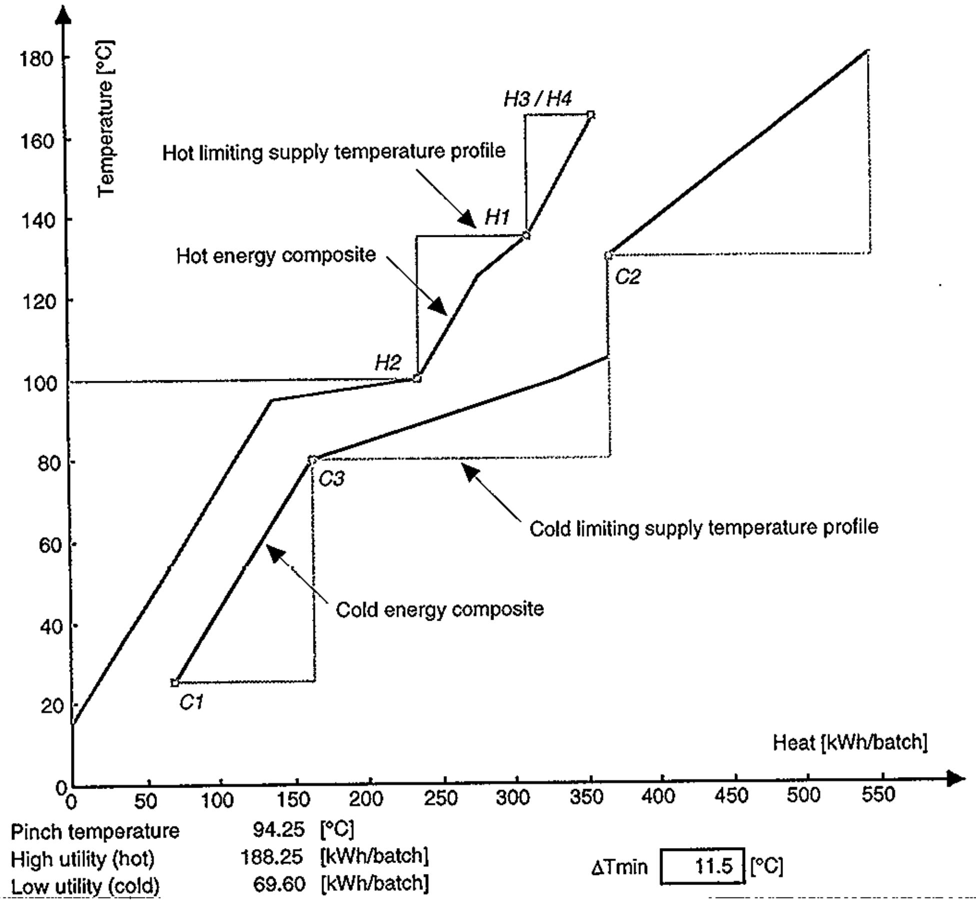


**Figure 2-4** Limiting supply temperature profiles - batch example process EP1 (refer to comments in the text).

### 2.2.3.2 Defining the Intermediate HSUs

Once the LSTP have been drawn, the minimum number of HSUs can be determined with respect to the cold composite (refer to *Figure 2-5*), i.e. starting from the cold end of the cold composite (which is also the cold end of the heat recovery region).

Then, the minimum number of HSUs with respect to the hot composite (i.e starting from the hot end of the hot composite and progressing downwards, refer to *Figure 2-6*) is determined. Of course, the minimum number of HSUs does not actually depends on the «search direction» (temperature upwards or downwards), but the boundary position (in term of energy coordinate) of storage units are different in general (e.g. compare the upper bound position of $HSU2_{ub}$ on *Figure 2-5*, with the lower bound position of $HSU2_{lb}$ on *Figure 2-6*).

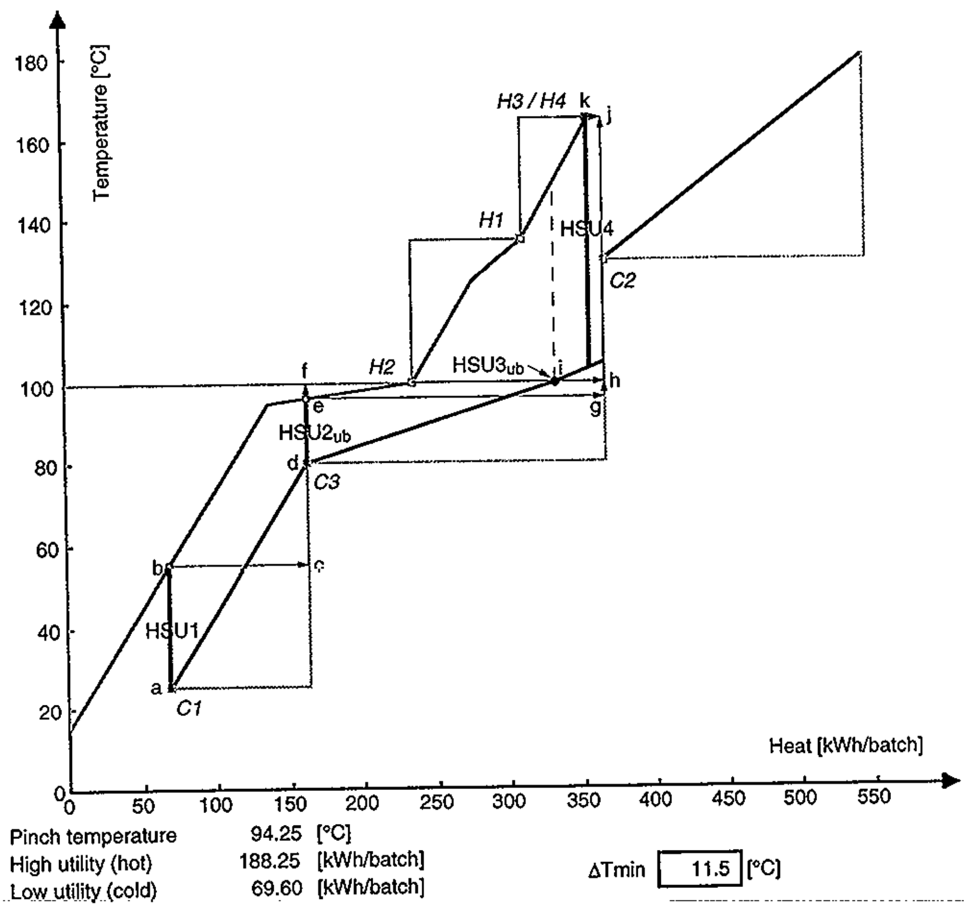


**Figure 2-5** Defining the upper boundary position and the minimum number of HSUs with respect to the cold energy composite - batch example process EP1 (refer to comments in the text).

The minimum number of HSUs, e.g. with respect to the cold composite, is determined according to the following rules (refer to *Figure 2-5*):

1. the first storage unit (HSU1) is of course assigned to the cold end of the heat recovery region (point a);
2. move vertically to the hot composite, defining the highest possible supply temperature of cold streams to be included in the storage sub-system (point b). Point b is not constrained by hot streams (actually it is never constrained, since it is the cold end of the heat recovery) and hence represents the absolute maximum operating temperature of HSU1. Therefore moving horizontally to the vertical segment of the cold LSTP (point c) defines all cold streams (if any) which supply temperature is compatible with the storage sub-system Sss1-2 and identify which cold stream requires the introduction of a new heat storage unit (in this case cold stream C3);

3. the cold LSTP segment can be extended to a vertical line, which intersects the cold (point d) and hot (point e) composites. This defines the location of HSU2 with respect to the supply temperature of the cold streams. Yet it remains to be verified whether the supply temperature of the hot streams are not more constraining than that of the cold streams (a case that would be encountered e.g. with a process including only one cold stream but several hot streams). This is checked by searching for the intersection of the vertical line passing through point c and the horizontal line passing through the first supply temperature encountered starting from point b (here hot stream H2);
4. if the intersection (point f) is above point e (i.e. above the hot composite), hot streams are not constraining at all, i.e. no hot stream starts in the identified storage sub-system Sss1-2. If the intersection is located between point e and d (i.e. in the inter-composite region), the hot streams constrain the operating temperature of HSU2, but not its location (heat recovery range). If the intersection is located below point d (more generally below the cold composite), the hot streams are more constraining than the cold streams, since they not only constrain the operating temperature of HSU2, but also its location, which has to be shifted on the left (see point 7) below for the procedure relevant to this case);
5. point f actually lies above point e, hence HSU2 can be kept as such. The operating temperature of HSU2 is not constrained on the hot side and point e represents the maximum operating temperature of HSU2, and hence moving horizontally to the vertical segment of the cold LSTP (point g) will define all streams (if any) which supply temperature is compatible with the storage sub-system Sss2-3 and identify which cold stream requires the introduction of a new heat storage unit (cold stream C2 in this case);
6. the vertical line passing through point g is outside the heat recovery range, indicating that HSU3 could maybe be located at the hot end of the heat recovery range and that minimum number of HSUs would be 3. But it remains to be verified whether the hot streams are not more constraining than the cold streams;
7. this is checked by searching for the intersection of the vertical line passing through point g and the horizontal line passing through the first (hot) supply temperature encountered starting from point e (here again hot stream H2). The intersection (point h) is located below the cold

composite, and the maximum «allowable» location of HSU3 is actually point i. If HSU3 is located at point i, its operating temperature is constrainted to be lower than or equal to the supply temperature of H2, while at the same time higher than or equal to the temperature of the cold composite at point i, i.e. the operating temperature of HSU3 is pinched on both sides;

8. moving again horizontally from the highest possible operating temperature of HSU3 (i.e. temperature of point i) to the cold LSTP defines point h again. But the intersection of the vertical line passing through h and the horizontal passing through the first (hot) supply temperature above (on the right) of HSU3 (H3/H4) defines point j, which is located «between» the composites but outside the heat recovery range. Therefore HSU4 can be located at the hot end of the heat recovery region, and point j (representing the maximum operating temperature of HSU4) be translated to point k;
9. finally, starting at the cold end, 4 HSU are required. The (possibly) constraining supply temperature of cold streams are accounted for by increasing the lower boundary of the temperature margin of storages. Such a case is not found here, since the lower boundary on the operating temperature of all HSUs is defined by the cold composite itself.

The same procedure can now be applied starting from the hot end, reversing the role of hot streams and cold streams (refer to *Figure 2-6*). Note that the numbering of HSUs is in the reverse order of placement, for easier comparison with the case resulting from the procedure starting from the cold end of the cold composite. Note also that H1 is contraining the maximum allowable temperature of Sto4, a case which was not found when defining the HSUs starting from the cold end of the heat recovery region (see former step 9).

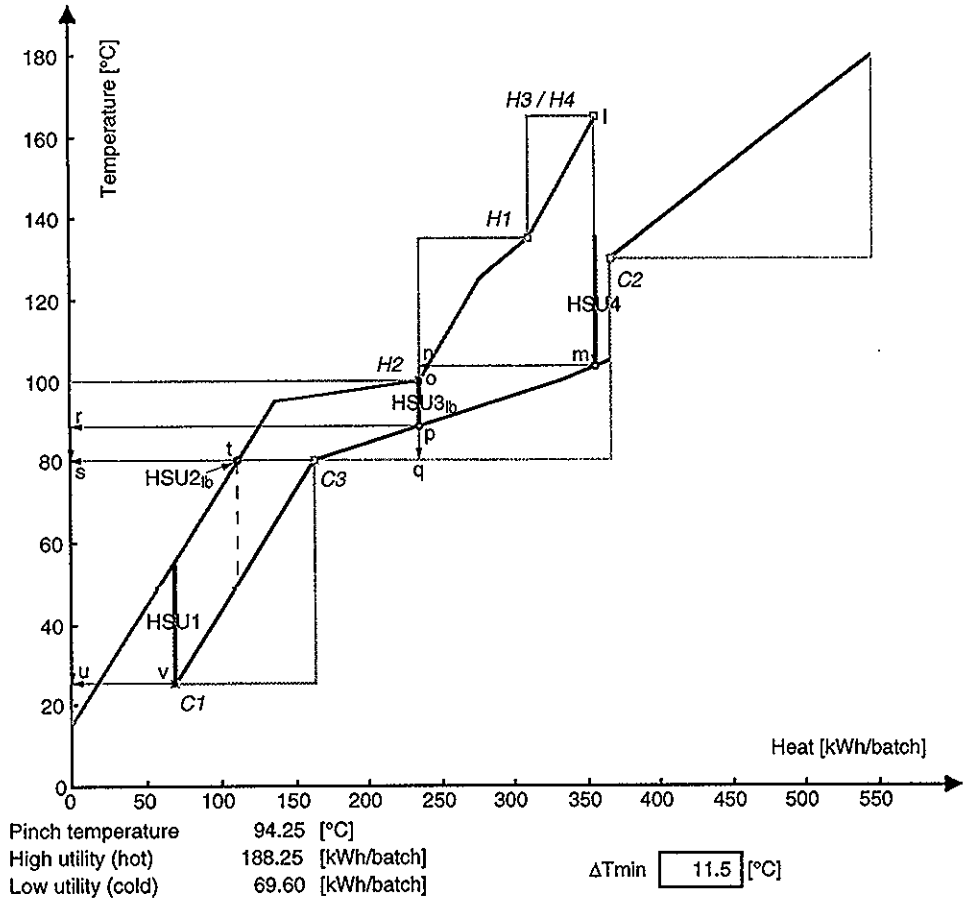


**Figure 2-6** Defining the lower boundary position and the minimum number of HSUs with respect to the hot energy composite - batch example process EP1 (refer to comments in the text).

### 2.2.3.3 Minimum Number of HSUs : Summary and Comments

Given a HR value, the minimum number of HSUs is independent of the starting point for their determination (cold end or hot end), as can be noticed from the above example (EP1).

The results of the former steps are summarised on *Figure 2-7*, showing that at least 4 HSUs are required for the chosen HR level. With respect to energy, the positions of HSU1 and HSU4 are fully determined, while HSU2 and HSU3 can be chosen between the two boundary positions previously identified, as highlighted. This degree of freedom can be used to mimimize capital costs, since e.g. HSU2 is fully pinched at its lower boundary position, while it benefits from a full (unpinched) temperature window if at its upper boudary position.

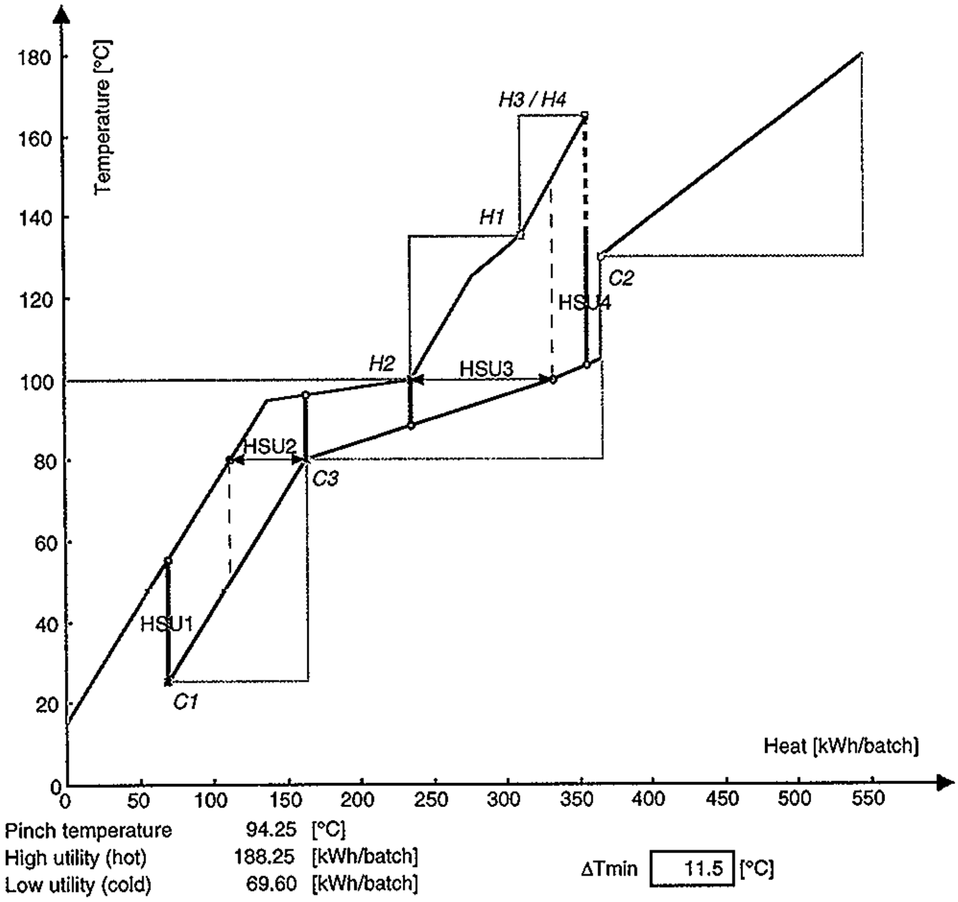


**Figure 2-7** Operating temperature and heat recovery margins of the minimum number of HSUs - batch process example EP1 (refer to comments in the text).

Note that in the present case, the energy ranges of HSU2 and HSU3 do not overlap, but this is not a general rule, as illustrated on *Figure 2-8*, which represents a brewery process. This demonstrates that intermediate HSUs can not be independently assigned any position within the identified range; in other words, once HSUn is assigned, the assignement of HSUn+1 has to take the assignment of HSUn into account (and so on for all intermediate HSUs). Refering to the brewery process, if HSU2 was assigned the HSU2ub position (although this would be a bad choice), HSU3 could not be assigned the HSU3lb position (or any other place on the left of HSU2).

When selecting the position of intermediate HSUs, the following aspects should also be taken into account:

1. to minimize the number of HEXs (i.e. avoiding the need to match a process stream with too many storage sub-systems), a storage should be assigned either at the end or at the start of a process stream. Assigning it

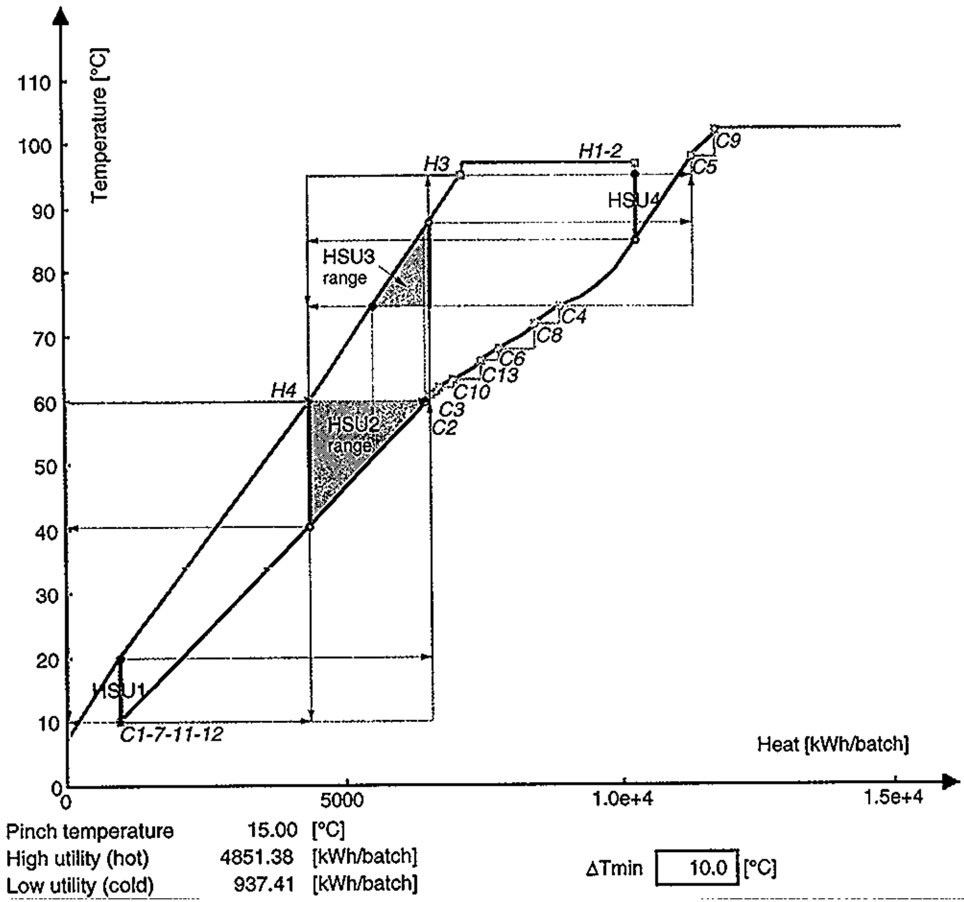


**Figure 2-8** Overlaped HSU assignment ranges (case of a brewery process).

at the supply temperature has the advantage of eliminating a possible constraint on the temperature margin of the storage; this is recommended at least when the constraint is «hard», while other effects should be taken into account if the temperature constraint introduced by the supply temperature is only «soft»;

2. the sequence of the sub-set of streams within each storage sub-system influences the storage capacity, and the capital costs. The possible magnitude of this effect remains to be assessed on the basis of case studies;

3. the heat recovery range of a storage sub-system (i.e. the position of intermediate HSUs) does not only influence the temperature window of intermediate HSUs, but also that of HSUs at the end of the HR region. E.g., HSU4 is not constrained when starting from the cold end, since hot stream H1 is included in the Sss2-3 sub-system, while HSU4 is constrained by H1 when designed starting from the hot end.

Based on the preceding comments, a reasonable assignement would be: HSU1 to C1, HSU2 to C3, HSU3 to H2, HSU4 to H3/H4. Assigning HSU3 to H1 to prevent H1 from constraining HSU4 would likely result in a sub-optimal solution, since the temperature margin of HSU3 would still be quite small (refer to *Sub-section 2.3.2* on page 51).

The proposed procedure, using a graphical representation and based on the assumption of «vertical» heat transfer between composites, provides the designer with the necessary insight for selecting HSUs:

- by systematically working from the cold end towards increasing temperatures, and from the hot end towards decreasing temperatures, respectively, the «energy margin» of each HSU, i.e. the range of energy coordinates the HSU can be located at, is easily identified;
- the LSTP plots help in identifying critical streams with respect to the definition of the minimun number of HSUs;
- the «temperature margin» as function of the actual assignment of the HSU within its «energy margin» is highlighted, allowing for some degree of freedom to be used for optimization;
- the relationship between the number of HSUs and the amount of HR is easily calculated and allows to identify critical values of HR where storage pinch(es) appear and hence topological traps are expected.

### 2.2.3.4 Extension of the Method for $\Delta T_{minSto}$>0 °C

So far, the calculation of the minimum number of HSUs for a given amount of HR assumes an absolute minimum $\Delta T_{minSto}$=0 °C. As already explained (refer to *Sub-section 2.2.2* on page 24), economic $\Delta T_{minSto}$ values of can be very small indeed.

However, a stream-wise $\Delta T_{min}$>0 may be required. In this case, the procedure is similar to the one for $\Delta T_{minSto}$=0 °C, previously described, but includes a preliminary step:

- define the stream-wise dependent $\Delta T_{min}$ (or select a constant $\Delta T_{min}$ value for all streams) and shift the stream temperatures accordingly (+$\Delta T_{min}$ for cold streams, -$\Delta T_{min}$ for hot streams);

then apply the previously described procedure on shifted composites (instead of «actual temperature» composites). Using shifted composites automatically garantees that the prescribed stream-wise dependent $\Delta T_{min}$ for heat transfert are satisfied.

Individual temperature shifting of streams can be a way to account for various parameters affecting the model of vertical heat transfer (counter-current heat exchanges) such as significant discrepancies between the heat transfert coefficients, between the duration of the streams (actual heat rate of HEXs), or other integer effects such as effect on sequence, etc. These issues should be further analysed and methods be proposed. The stream-wise dependent $\Delta T_{min}$ could be calculated based on the «optimum» situation obtained without $\Delta T_{min}$ shifting, which could serve as the reference case for the available driving forces, etc. Stream-wise dependent $\Delta T_{min}$ will «reorganize» the stream population within each storage sub-system; but it remains to be verified that the discretization of the problem due to the finite number of storage levels (storage sub-systems) does not mask fine tuning effects due to the optimization of the heat contribution of streams within each sub-system.

The effect of specifying a stream-wise $\Delta T_{minSto}$ value on the minimum number of HSUs can also be assessed.

#### *2.2.3.5 Optimization Opportunities*

As already mentionned, the proposed procedure for defining the minimum number of HSUs is based on the simplifying assumption of «vertical heat transfer», i.e. the vertical definition of heat storage sub-systems. This is a «default best guess» and is the only case where a straightforward, simple application of the method is possible, leading to results of suitable precision at the preliminary design stage (quite similar to the vertical heat transfer assumption used in continuous processes for targeting the minimum area requirement).

The following opportunities to reduce the number of HSUs below the minimum number of HSUs as predicted by the proposed method require this simplifying assumption to be removed:

- criss-cross heat exchanges at the border between two heat storage sub-systems (vertical separation line), e.g. remaining heat from a hot stream normally supplied to the lower storage sub-system is supplied to the upper sub-system, while heat at the beginning of a cold stream (from the supply temperature) normally supplied by the lower sub-system is provided by the upper heat storage sub-system (refer to *Figure 2-15* on page 56). This allows the heat recovery to be increased beyond the maximum amount of HR feasible with a given number of HSUs (according to vertical model) without requiring an additional HSU to be introduced. The number of HEXs is also reduced, while these benefits are at the expense of decreasing the temperature margin of the concerned HSU;

- eliminating from HR consideration some small streams which supply temperature is in, but close to the end of, the HR region. This prevents the operating temperature of an intermediate HSU to be pinched, while the temperature margin of the related HSU at the border of the HR region decreases. This is actually equivalent to trading-off the temperature margin of one HSU against another one;
- it is even possible to remove from HR consideration some small streams fully included in the heat recovery region if these streams require an intermediate HSU to be introduced. In this way, the required number of HSUs decreases, at the expense of smaller temperature driving force, hence of increased heat transfer area. Hopefully the economics improves. Such an opportunity is seldom used in continuous processes, since the process pinch has a major effect on the capital costs, while in batch processes optimum solutions are often to be found at the transition regions between two numbers of HSUs, i.e. effects other than the process pinch come into play.

The above opportunities actually correspond to criss-cross heat exchanges, which are known to increase the necessary HEX area in most cases. Hence they exploit trading-off HSU capital costs against HEX area.

Note also that the last two opportunities have already been mentionned independently by Sadr-Kazemy & Polley (1996), and by Stolze *& al.* (1995). However, the measures were not discussed and assessed on the basis of a graphical representation of the minimum number of HSUs.

### 2.2.4 Stream-wise or Slice-wise Supply Temperatures ?

So far, the supply temperature of all process streams have been taken into account in the «limiting supply temperature profiles» (LSTPs). This is equivalent to assuming that all streams are independently scheduled and completely asynchronous with any other streams, so that, during a batch cycle, there is (or there might be, in the case of schedule variations likely to take place) a time period for the supply temperature of each cold stream to be the lowest temperature of all cold streams present, and a time period for the supply temperature of each hot stream to be the highest temperature of all hot streams present at that time period. In other words, all supply temperatures are deciding (this condition will be made clear below when analysing the EP1 example process). This is a sound assumption, since robust solutions, insensitive to schedule variations, are searched for. It leads to the most constrainted «limiting supply temperature profiles» and the largest minimum number of HSUs.

However:

- groups of related, synchronous streams exist (named «master / slave» groups of streams);
- the number of time slices is often in the order of, or smaller than, the number of process streams. Based on the rules proposed for storage assignment on the batch cascade curves (BCC) (Krummenacher & Favrat, 1995), a restricted set of «deciding» supply temperatures can be established.

Both cases often result in relaxed LSTPs, and a smaller number of HSUs, as will be demonstrated below. But care must be taken so as to verify the feasibility of the heat exchanges.

#### 2.2.4.1 Master/Slave Groups of Streams

Master/slave groups of streams describe a fundamental relation of cause and effect between the streams, so that simultaneity of streams is guaranteed in any case. If the master stream (the cause) is delayed, the slave streams (he effect) are delayed as well.

If several hot streams (several cold streams, respectively) are included in the same M/S group, only the hot stream with the highest supply temperature (the cold stream with the lowest supply temperature, resp.) is deciding, the supply temperature of other streams in the same M/S group being «overlaid» or «wiped off». In this way, the LSTPs are relaxed and this generally results in a smaller number of HSUs for a given amount of HR.

### 2.2.4.2
### *Time Slices*

Originally, the analysis of the stream-wise versus the slice-wise approach to the number of HSUs was motivated by experience gained from batch cascade curves (BCCs) (refer to Krummenacher & Favrat, 1995). In BCCs, the existence of process streams disappears since BCCs are built from the grand composite curve of each time slice. The number of time slices is deciding for the number of «supply temperatures», while in the stream-wise approach the number of streams defines the number of supply temperatures. For the problem at hand, the number of time slices (which may range from twice the number of process streams in the worst case to 1 if all streams are synchronous, hence equivalent to a continuous process) is not actually the only deciding variable. Consider example process EP1 (refer to *Figure 2-1* on page 18 and *Table 2-1* on page 19). The supply temperatures of each time slice (i.e. the starting temperature of the cold and the hot time slice composites) are summarized in *Table 2-2*.

| Time Slice | Cold Comp. $T_{supply}$ | Hot Comp. $T_{supply}$ |
|---|---|---|
| 1 of 5 | C1: 25 °C | – |
| 2 of 5 | C1: 25 °C | H1: 135 °C |
| 3 of 5 | C1: 25 °C | H3/H4: 165 °C |
| 4 of 5 | C1: 25 °C | H1: 135 °C |
| 5 of 5 | C3: 80 °C | H3/H4: 165 °C |

**Table 2-2** The cold and hot supply temperatures of each time slice - batch example process EP1.

Globally, there are 2 different cold supply temperatures, and 2 different hot supply temperatures, hence 4 supply temperatures for 6 process streams (H3/H4 actually counts for one single stream). It is as if streams C2 and H2 were not deciding. Such «idle» streams are easily identified on the time event model of *Figure 2-9*, redrawn from *Figure 2-1* on page 18, according to the following rules:

- hot streams are grouped together, and so are cold streams too;
- hot streams are listed by decreasing order of supply temperature;

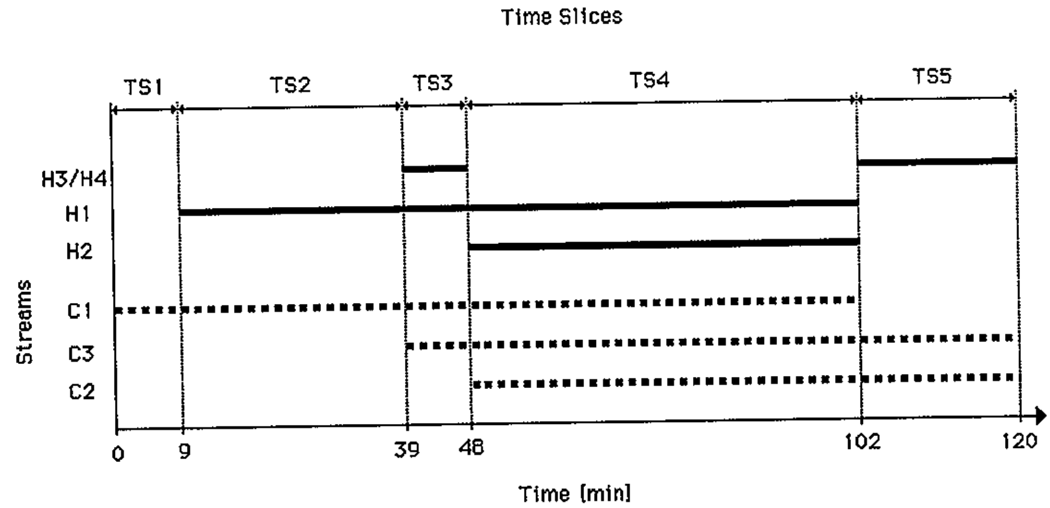


**Figure 2-9** Time event model of example process EP1, organized so as to highlight streams that are overlaid both in time and temperature.

- cold streams are listed by increasing order of supply temperature.

It becomes clear that whenever C2 exists, a cold stream with a lower supply temperature (C3) also exists; similarly, whenever H2 exists, a hot stream with a higher supply temperature (H1) also exists. However, in this particular case, the «wiping off» effect of C2 is sensitive to schedule variations affecting the stop time of C3 with respect t that of C2. The same is true for H1 with respect to H2, although H4 might help overlap H2 if the stop time of H2 is delayed.

Hence, removing the supply temperatures of C2 and H2 from the list of supply temperatures to be taken into account in the LSTPs is not recommended, unless sufficient time margins can be guaranteed.

Compared to the case represented on *Figure 2-7* on page 34, if C2 and H2 are actually removed from the list of deciding streams, the minimum number of HSUs is reduced from 4 to 3, as illustrated on *Figure 2-10* when starting from the cold end, and on *Figure 2-11* when starting from the hot end. This reduction is due to the elimination of H2, since C2 is not included in the HR region anyway and therefore is not constraining the LSTPs.

In both figures, the solid line joining HSU2 to HSU3, represents the actually highest operating temperature of HSU3 for the given operating temperature of HSU2. Above this line, the heat exchanges during time slice 4 are not feasible (e.g. dotted line).

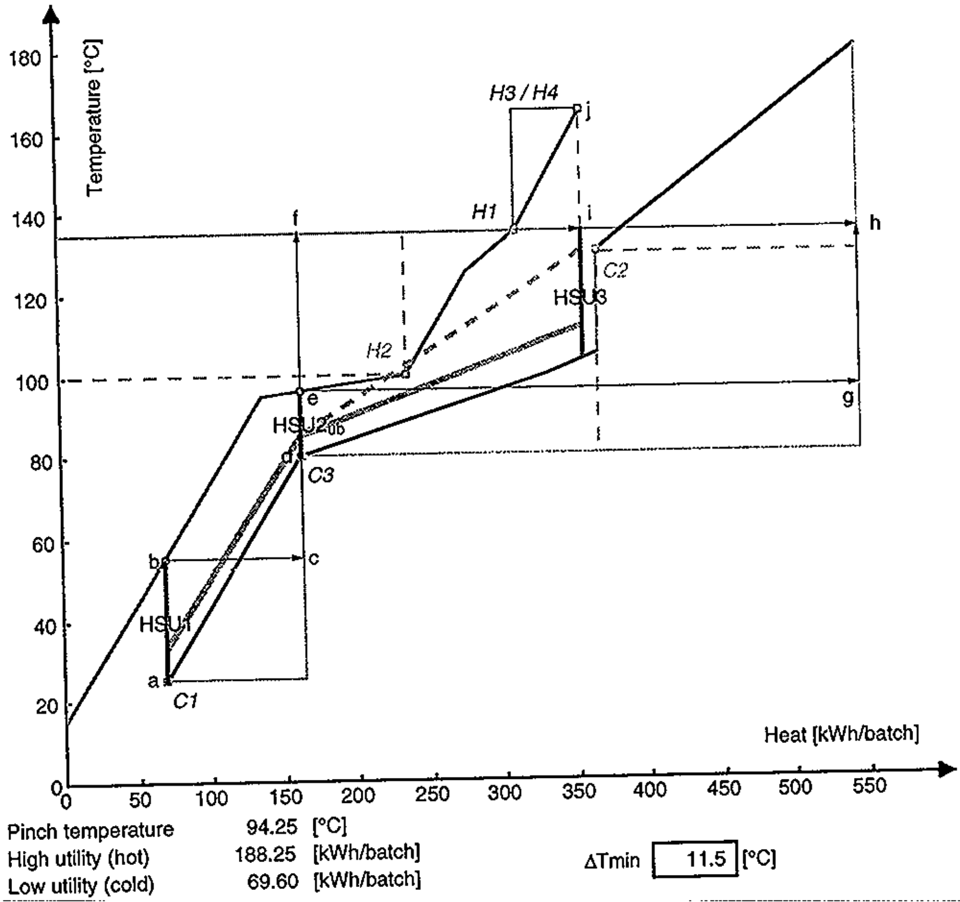


**Figure 2-10** The minimum number of HSUs without taking the supply temperature of H2 (and C2) into account, starting from the cold end (same HR as *Figure* 2-7 on page 34).

Formerly, accounting for the supply temperature of each process stream (assuming single segment streams only) in the LSTPs guaranteed that the temperature driving forces of individual process stream - storage streams matches be feasible in practice. Such a guarantee does not exist anymore if «composite process streams» (i.e. having a composite temperature profile which has not a constant $\dot{M}c_p$ anymore, resulting from some streams being «wiped off» from the list of deciding streams) are to be matched with storage streams. Infeasible matches cannot be identified at a glance from the TAM energy composites, which compose streams which do not coexist at the same time.

If the time schedule of streams theoretically allows some «idle» streams to be removed, this can however lead to situations where intermediate HSUs need to be introduced so that the «storage composite» remain between the process TAM composites (a «storage composite» has to be a straight line

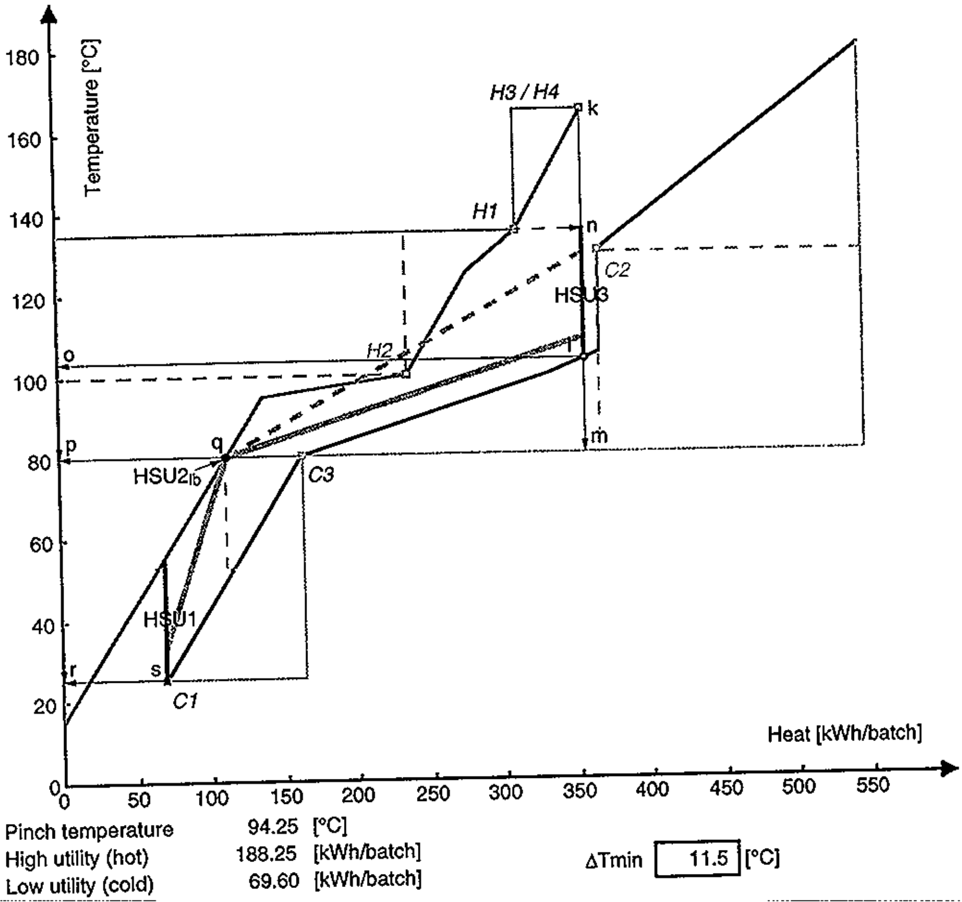


**Figure 2-11** The minimum number of HSUs without taking the supply temperature of H2 (and C2) into account, starting from the hot end (same HR as *Figure 2-7* on page 34).

between two HSUs). This is a new situation due to «composite process streams» existing during time slices, which was not found in the basic situation of stream-wise approach to LSTPs (where all convex points of the process composite - these are problematic with respect to the feasibility of «composite streams» - are associated to supply temperatures of process streams and reflected in the LSTPs).

Hence the TDF feasibility of such matches during the related time slices has to be individually checked. If an infeasibility appears, an intermediate HSU has to be included. A reasonable guideline for introducing an additional HSU states: first check the feasibility for all concerned streams, list infeasible matches, and only then decide where additional HSUs are best introduced.

Summarizing the opportunities for the minimum number of HSUs to be reduced:

- provided that the time event model of process streams is organised according to the above simple rules, this representation also allows for an easy visual check of any «undeciding», «idle» streams. A sensible strategy is to first take all streams into account to draw the LSTPs and defines the «by-default» minimum number of HSUs. Then identify constraining (critical) streams and check on the time event model whether their supply temperature could be removed from the LSTPs, while sufficient time margin is guaranteed (supplementary data should be provided to model worst case arising from likely schedule variations (remains to be developed).
- the feasibility of matches including «composite process streams» has to be individually verified, and the design of the HEN has to be time slice oriented (at least for the «idle» streams);
- the elimination of some «idle» streams based on the time slice approach can lead to more cost-effective design, at the expense of more complex HEN, since serial, or serial / parallel HEN configurations are required to avoid intermediate HSUs, which is not the case of streamwise HSU assignment, where only single, one-to-one matches are present;
- the strategy towards optimally selecting HSUs is, like Pinch Analysis for continuous processes, basically an iterative procedure.

## 2.3 Search for Optimum 100% Indirect HR Schemes

The search for cost optimum 100% indirect heat integration solutions can be addressed using several approaches. The corresponding mathematical model is worth a description since this model is quite simple, and also because it is needed for a GA based optimization (refer to *Sub-section 2.3.3* on page 62). The heuristic approach, based on Pinch Analysis and using the various graphical tools and methods formerly presented, has the advantage of both being feasible and maybe more importantly, providing insight in the problem, although it is certainly not possible to demonstrate that a better solution couldn't be found !

### 2.3.1 Mathematical Model

It has formerly been mentionned that the design of indirect HR schemes is much simpler than that of direct HENs (for continuous or batch processes). In fact, while the structure (topology) of continuous HENs is an issue as important as the heat rate of the matches, this is generally not an issue for indirect HENs, at least not with the sensible assumptions mentionned below, which almost fully define the structure, i.e. heat exchangers are «organized» around the HSUs.

#### 2.3.1.1 Assumptions

The following sensible assumptions make the derivation of the model particularly easy:

1. arrangement of the HSUs into serially interconnected storage sub-systems, each storage sub-system associated with two adjacent HSUs being mass and heat balanced over a batch cycle time. These conditions are refered later as «cyclic serial operation»;
2. within each sub-system, each process stream feeding heat to (or supplied by) the heat storage is matched to the related heat storage by a single HEX unit, since the $\dot{M}c_p$ of storage streams can be adjusted as needed;
3. the determination of the number of HSUs takes the supply temperature of all process streams into account.

#### 2.3.1.2 Comments

In essence, the above assumptions exclude mixing of HSUs for mass balancing their content, and heating /cooling them by external utilities for heat balancing. This is so because mixing of storages fluid wastes temperature driving forces, and hence HEX area and HSU capacity (refer to Krummenacher & Auguste, 1997). It could be compensated by savings arising from a reduced number of HEXs units (both process and utility units, refer to Mikkelsen, 1998). The actual effect of this trade-off (which cannot be assessed at this stage) depends on the considered cost functions of HEXs. In this respect, it should be noted that the serial arrangement of HEX units on one process stream would often not be significantly more expensive than a single overall unit (e.g. for plate & frame HEXs). At least, assuming a large initial cost of HEX units is clearly invalid in this case.

At this stage, the assumption of the cyclic serial operation is preferred since it allows for a simpler optimization model.

The third assumption further simplifies the HEN structure by making it independent of time slice, since if some «idle» streams were not taken into account in the definition of the HSUs, a serial-parallel, time dependent HEN sub-structure would be needed (refer to *Sub-section 2.2.4* on page 38).

### 2.3.1.3 Indirect HR Structure

Under the above assumptions, the structure of the HR scheme would schematically be as depicted on *Figure 2-12.*

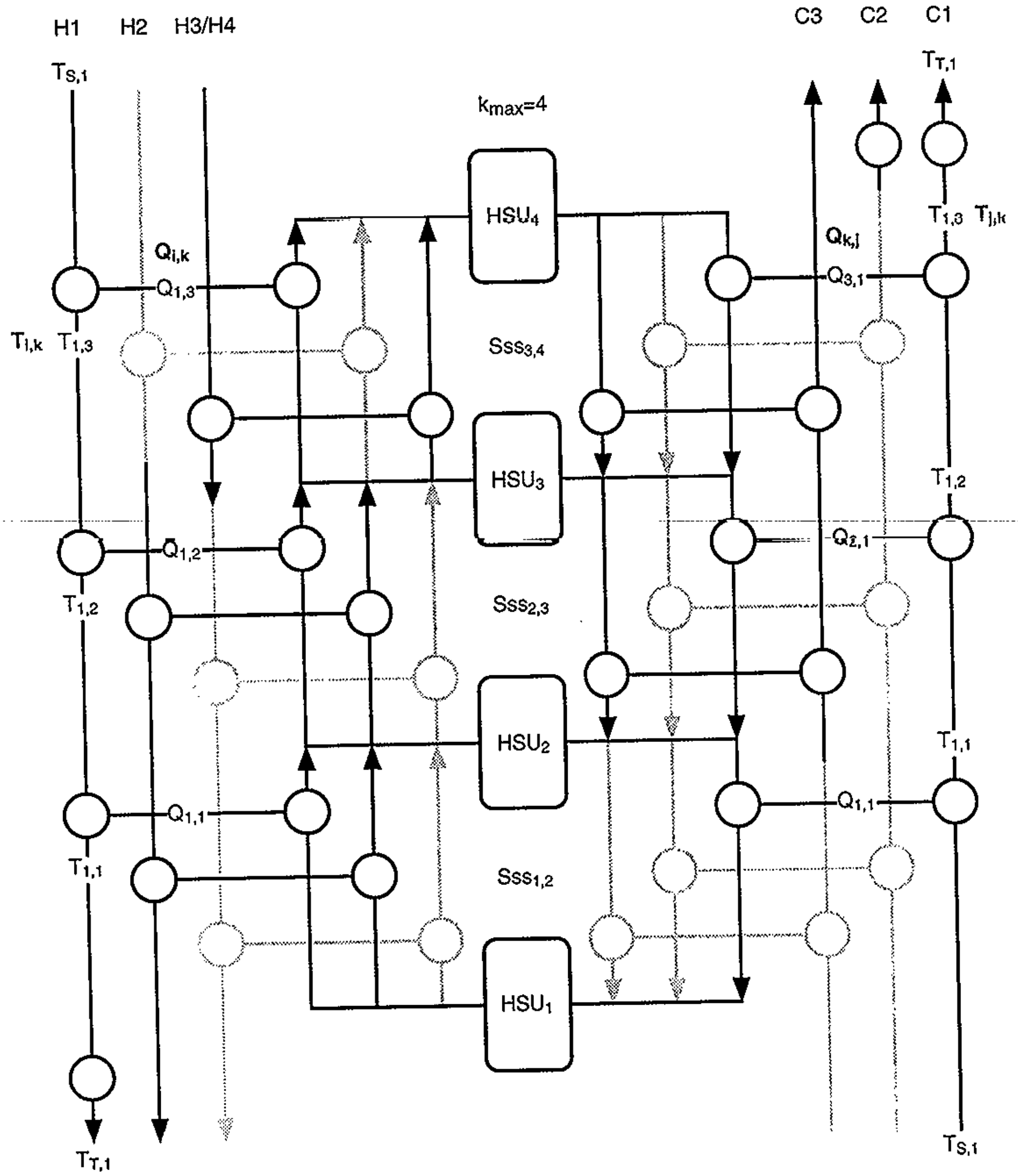


**Figure 2-12** Schematic HR scheme deriving from the assumptions mentionned above - batch process EP1, conditions of *Figure 2-2* on page 20.

### 2.3.1.4 Problem Statement

Given:

- a batch process and its related economic data and costs functions;
- a number of HSUs specified by the user;

determine:

- the operating temperature of the HSUs;
- the heat rate of each of the process-heat storage stream matches (HEXs from the HEN structure);
- the corresponding overall heat recovery;

which minimize the specified economic criteria (e.g. TACs, NPCs, etc.).

### 2.3.1.5 Mathematical Formulation

Let's define (refer to figure *Figure 2-12*):

- HPS be the set of the hot process streams (subscript $i$); $i : 1 .. I$ );
- CPS be the set of the cold process streams (subscript $j$); $j : 1 .. J$ );
- HSU be the set of the heat storage units (subscript $k$; $k : 1 .. K$ where $K$ is the number of HSUs);
- $Q_{i,k}$ be the heat feeded from the hot process stream $i$ to the storage stream coming out from $HSU_{k-1}$ into $HSU_k$;
- $Q_{k,j}$ be the heat supplied to the cold process $j$ by the storage stream coming out from $HSU_k$ into $HSU_{k-1}$;
- $T_{i,k}$ be the temperature of the hot process stream $i$ after heat exchange with the storage sub-system $Sss_{k,k+1}$ (i.e. consisting of $HSU_k$ and $HSU_{k+1}$), while $T_{S,i}$ denotes the supply temperature of the hot stream $i$ and $T_{T,i}$ denotes its target temperature;
- $T_{j,k}$ be the temperature of the cold process stream $j$ after heat exchange with the storage sub-system $Sss_{k,k+1}$ (i.e. consisting of $HSU_k$ and $HSU_{k+1}$), while $T_{S,j}$ denotes the supply temperature of the cold stream $j$ and $T_{T,j}$ denotes its target temperature.

In order to keep the notation general, it is assumed that a match potentially exists between each process stream and each storage sub-system, irrespective of the corresponding temperatures. In case of reverse TDF, the heat load of the match will be set to zero, i.e. the match does not exist.

The variables of the problem are the following:

- the heat contributions $Q_{i,k}$ and $Q_{k,j}$. An alternate choice could be the heat rate $\dot{Q}_{i,k}$ and $\dot{Q}_{k,j}$, or the «cut-off» temperatures of the process streams after heat exchange with each storage sub-system $T_{i,k}$ and $T_{j,k}$. The exact choice does not matter, since these variables are linearly related to each other;
- the operating temperature of the HSUs $T_k$.

The variables of the problem are subject to the constraints of:

1. monotonically increasing temperature of HSUs, expressed by:

$$T_k > T_{k-1} \quad \forall k \in HSU \tag{2-1}$$

where:

- $T_{minCC} \leq T_k \leq T_{maxHC} \quad \forall k \in HSU$
- $T_{minCC}$ is the minimum temperature of the cold composite curve (the minimum of the supply temperature of the cold streams);
- $T_{maxHC}$ is the maximum temperature of the hot composite curve (the maximum of the supply temperature of the hot streams).

2. overall mass balance of each HSU over a batch cycle time (the energy balance is automatically satisfied if the heat losses to ambient can be neglected).
The mass balance of an intermediate $HSU_k$ depends on both the storage sub-systems $Sss_{k-1,k}$ and $Sss_{k,k+1}$ («full mass balance»), while the mass balances of the first and the last HSUs in the «storage chain» only depend on one storage sub-system («half mass balance»). But since «full mass balances» are actually made of two «half mass balances» of the adjacent storage sub-systems, each of the «half mass balances» has to be individually satisfied, leading to the following conditions:

$$\frac{1}{c_{p_k}(T_k - T_{k-1})}\left(\sum_i Q_{i,k} - \sum_j Q_{k,j}\right) = \sum_i M_{ki} - \sum_j M_{kj} = 0 \quad \forall k \in HSU \tag{2-2}$$

and since $T_k$ and $T_{k-1}$ are assumed to be constant and $T_{k-1} < T_k$, *Equation 2-2* can be simplified as the following simple constraints:

$$\sum_i Q_{i,k} - \sum_j Q_{k,j} = 0 \quad \forall k \in HSU \tag{2-3}$$

3. feasibility of heat transfer, i.e. positive temperature driving forces (else $Q = 0$ for $k_i > k_{imax}$, $k_i < k_{imin}$ or $k_j < k_{jmin}$, $k_j > k_{jmax}$ as described below).
   These constraints can be written as:

$$T_{i,k} < T_k \text{ for the hot process streams} \tag{2-4}$$

and

$$T_{j,k} < T_{k+1} \text{ for the cold process streams} \tag{2-5}$$

Introducing the variables $Q_{i,k}$ and $Q_{k,j}$, the above conditions result in the following constraints:

$$T_{i,k+1} - \frac{Q_{i,k}}{M_i c_{pi}} > T_k \quad \text{for all } k_i \text{ with } k_{imin} \le k_i \le k_{imax} - 1 \tag{2-6}$$

where:

- $k_{imin}$ is defined by the smallest $k_i$ satisfying $T_{T,i} < T_{k_{imin}}$ while $k_{imin} \ge 1$
- $k_{imax}$ is defined by the largest $k_i$ satisfying $T_{S,i} > T_{k_{imax}}$ while $k_{imax} \le K$
- $T_{i,k+1} = T_{S,i}$ for $k_i = k_{imax} - 1$

and

$$T_{j,k-1} + \frac{Q_{k,j}}{M_j c_{pj}} < T_{k+1} \quad \text{for all } k_j \text{ with } k_{jmin} \le k_j \le k_{jmax} - 1 \tag{2-7}$$

where:

- $k_{jmin}$ is defined by the smallest $k_j$ satisfying $T_{S,j} < T_{k_{jmin}}$ while $k_{jmin} \ge 1$
- $k_{jmax}$ is defined by the largest $k_j$ satisfying $T_{T,j} > T_{k_{jmax}}$ while $k_{jmax} \le K$
- $T_{j,k-1} = T_{S,j}$ for $k_j = k_{jmin}$

4. non-negativity of the heat contribution variables $Q_{i,k}$ and $Q_{k,j}$:

$$Q_{i,k} \ge 0 \tag{2-8}$$

and

$$Q_{k,j} \geq 0 \tag{2-9}$$

5. heat balance of the process streams:

$$\sum_k Q_{i,k} \leq M_i c_{pi}(T_{S,i} - T_{T,i}) \quad \text{for the hot process streams} \tag{2-10}$$

and

$$\sum_k Q_{k,j} \leq M_j c_{pj}(T_{T,j} - T_{S,j}) \quad \text{for the cold process streams} \tag{2-11}$$

These constraints prevent the target temperature of the process streams to be exceeded, which would result in unpromising solutions to be proposed. Reverse utilities would be needed - cold utility for cold streams, hot utility for hot streams - so as to bring back the final temperature of the streams to their target temperature.

The objective function to be minimized (e.g. the TACs economic criteria) can be expressed as:

$$C_{OpUtil} + [C_{CapHEX} + C_{CapHSU}] \cdot amort \tag{2-12}$$

where:

- $C_{OpUtil}$ is the annual cost of utilities, which is linear in the variables $Q_{i,k}$ and $Q_{k,j}$ ;
- $C_{CapHEX}$ is the capital cost of HEX units, which is non-linear in the variables (non-linearity arising from both the $\Delta T_{lm}$ found in the HEX area and the cost function of HEXs);
- $C_{CapHSU}$ is the capital cost of HSU units, which is non-linear in thevariables (non-linearity arising from both the capacity calculation and the cost function of HSUs);
- $amort$ is the annual amortization (pay-off) factor.

The above problem defined by *Equations 2-1 to 2-3, 2-6 to 2-11* (constraints), and *2-12* (objective function) is a NLP problem. All the constraints are linear with respect to the variables, while the objective function is non-linear.

Other important mathematical features of this NLP problem (e.g. convexity) have not been studied yet, so that it cannot be guaranteed that existing solvers shall be able to identify the global optimum.

Cost functions for HEXs and HSUs which include an initial costs factor are expected to introduce computational difficulties around zero because of the related discontinuity (since we require the cost to be zero if the HEX area or the HSU capacity are zero). The introduction of a multiplying exponential function could remove this problem.

However, considering the fact that the number of HEX units is not fixed, the objective function is very likely non-convex, preventing mathematical solvers to identify the global optimum. Only local optimums could be identified - but practical experiments with commercial solvers should be a achieved to verify this assertion.

Alternate solution approaches include a GA based optimization, which can use the above mathematical model (as described in *Sub-section 2.3.3* on page 62), and a heuristic, Pinch Analysis based approach, which is described next.

### 2.3.2 Pinch Analysis Approach

Since the proposed procedure derives from observations and understanding of the heat integration of test cases (in particular of EP1), it is meaningfull to first describe and comment these results before making them into a systematic procedure. Since the development of the «PinchLENI Java» version failed to provide the necessary tools for implementing the procedure, the basic steps have been calculated using an Excel worksheet.

#### *2.3.2.1 Indirect Integration of EP1*

The TACs have been systematically calculated for indirect heat integration of example process EP1, assuming 2, 3 and 4 HSUs, while the amount of heat recovery was varied. All supply temperatures of process streams have been taken into account. The operating temperatures of the HSUs have been optimized using the Solver Tool of Microsoft Excel. Considering *Figure 2-1* on page 18, it appears that the re-use of HEX units is not an issue in this case, except for H3 and H4, which are supposed to have the same location.

*Figure 2-13* represents the results obtained assuming a «vertical model», i.e. where the heat recovery range of the storage sub-systems, and the related cut-off temperatures of process streams, were vertically defined on the TAM composites. *Figure 2-13* deserves the following comments:

- the utility costs are drawn for reference (capital costs of utility HEXs are not included). Accounting for capital costs, an optimum (minimum) of

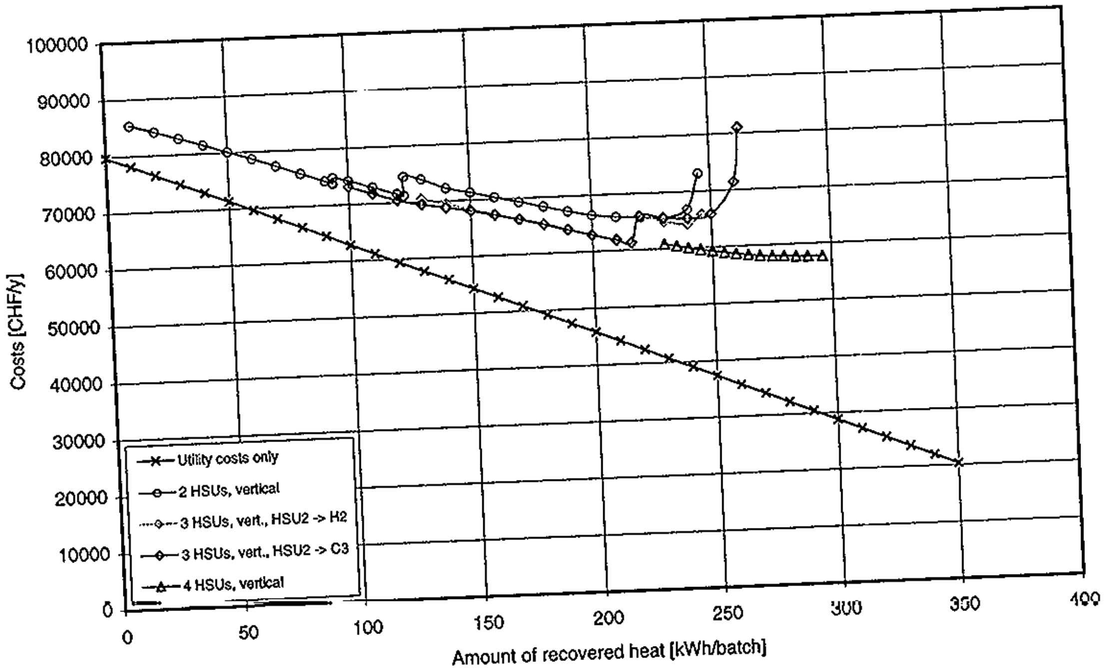


**Figure 2-13** Total annual costs of indirect heat recovery - example process EP1 with 2, 3 and 4 HSUs in vertical model (refer to text for further comments).

TACs is reached when the increase of annual capital costs as a function of the HR is equal to the decrease of the annual utility costs;

- with 2 HSUs, there is no alternate way to assign these units. The first step change of the TACs taking place at HR=93.5 kWh/batch is produced by the introduction of C3 in the heat recovery region, which heavily constraints the temperature of HSU1 (before C3 is introduced, the optimum temperature of HSU1 is much below 80°C). This new constraint results in increased HEX and HSU costs. Note that the introduction of H1 in the heat recovery region does not produce a step change, since the operating temperature of HSU2 is already at 135°C before H1 is introduced. The step change at HR=122.7 kWh/batch is due to the introduction H2, which constraints the temperature of HSU2 to suddenly change from 125 to 95°C. Then the TACs continue to decrease smoothly, encounter a minimum, until the absolute maximum limit at HR=246.75 kWh/batch is reached. At this point, the margin on the operating temperature of HSU1 falls to zero, because the cut-off temperature of the heat recovery region on the hot composite decreases below 80°C if the HR is increased (the lower limit of 80°C is required by C3). Even if the HR could be increased beyond this value, HSU2 would soon be pinched (actually for HR=262.5 kWh/batch) because the cut-off temperature of the heat recovery region on the cold composite increases above 100°C if the HR is increased (the upper 100°C limit on HSU2 is required by H2);

- assuming 3 HSUs, it has to be define «where» the intermediate HSU (now HSU2) has to be assigned. The introduction of an intermediate HSU should allow to further increase the heat recovery (and decrease the costs) by removing unfeasible temperature constraints on HSUs. From the case with 2 HSUs, it is clear that H2 and C3 are two constraining streams within the HR region (the LSTP plots outlined in *Sub-section 2.2.3* on page 27 would make this obvious). From a HR point of view, C3 is more constraining than H2, since with two HSUs, the bottleneck is first encountered on HSU1, which lower temperature limit is defined by C3, while the pinch on HSU2, linked to H2, would only become active for a higher HR. But the HR point of view is not necessarily in line with the minimum TACs, so that both cases - intermediate HSU2 assigned to C3 or HSU2 assigned to H2 - have to be assessed. Assigning an intermediate HSU to the start of a stream, i.e. to a supply temperature (rather than at any other position) is the most sensible choice, since the primary aim of introducing an intermediate HSU is to avoid a supply temperature from producing a bottleneck. This rule holds at least for the «vertical heat transfer» assumption. Once the decision concerning the assignment of HSU2 has been made, the TACs are calculated for various HR values. As a rule, the TACs calculations should restart from a HR value which makes the introduction of the new intermediate HSU feasible, and not only for HR values larger than the limit reached with one less HSU. With HSU2 attached to C3, a step change appears at HR=216.175 kWh/batch. Below this HR value, the supply temperature of H2 is on the left with respect to the one of C3 (i.e. heat from H2 is entirely recovered in the storage sub-system Sss1-2), while above this HR value, part of H2 is also integrated with Sss2-3, which requires the upper bound on the temperature of HSU to suddenly change from 135°C to 100°C (the actual, optimized operating temperature changes from 126.2°C to 99.8°C). The absolute upper bound to HR with HSU2 attached to C3 is HR=262.5 kWh/batch (defined by HSU being fully pinched at 100°C). A similar behavior is observed for HSU2 attached to H2, with a sudden change of the lower bound on HSU1 at HR=216.175 kWh/batch, changing from 25°C to 80°C (the actual, optimized operating temperature changes from 40.9°C to 80.2°C). But since HSU2 is assigned to H2 and not to C3, which is responsible for HSU1 being fully pinched first in the case of 2 HSUs, the the absolute upper bound to HR is unchanged at HR=246.75 kWh/batch. Despite the fact that the maximum HR is not significantly increased, the temperature margin of one of the two HSUs being pinched around the minimum TACs is relaxed, allowing the minimum TACs to be reduced by 6.6%. Note that assigning HSU2 to C3 or H2 leads to very similar TACs, but this effect is particular to this process;

- introducing a fourth HSU should allow to further increase the HR and hopefully decrease the TACs. From the former discussion for the case of 3 HSUs, the obvious decision is to assign the intermediate HSU2 to C3, and the second intermediate HSU3 to H2. The TACs slightly decrease as the HR increases, until an absolute maximum limit of HR=296.25 kWh/batch. Before this point, none of the for HSUs is going to be pinched, and the TACs continue to decrease slightly. But for HR>296.25 kWh/batch, the introduction of C2 in Sss3-4 makes HSU3 infeasible (a fifth HSU should be used). The heat integration including four HSUs features a further improvement of the TACs (compared to the 3 HSUs case) of 6.3%, with a simultaneous increase of the HR of 27%;
- a five HSUs heat recovery system has not been considered, due to the tedious, lengthy case-to-case implementation in an Excel Worksheet. But the principles are unchanged. Maybe a slightly improved TACs minimum could be found.

The above cases make use of the degrees of freedom 1) to 4) mentionned under *Sub-section 2.1.2* on page 18, i.e.:

1. the amount of HR (or the process $\Delta T_{min}$);
2. the number of HSUs;
3. the assignement of the HSUs (the definition of the storage sub-systems);
4. the operating temperature of each of the HSUs.

Degrees of freedom which remain to be used to potentially improve the solutions are the following:

5. the «cut-off» temperature of each process stream with each storage sub-system, to allow for an increase of the HR without encountering new constraining supply temperatures, or to decrease the capacity of HSUs by matching streams showing (on the average) good synchronism;
6. the rescheduling of streams to decrease the capacity of a «critical» HSU. This can be done using the procedure proposed in *Section 2.5* on page 70 and is not discussed later. As a preliminary, the rescheduling opportunities

(if any) associated with each process should be specified, and the critical HSU(s) have to be identified. Given the generally complex cause and effect links between tasks (streams), it is doubtfull that a systematic, simultaneous optimization of the heat recovery and the schedule be possible. Rescheduling does not only requires a set of binary or integer decisions to be made, since the delay, the advance, the new of mass flowrate, etc, need to be decided as well. Considering rescheduling requires an iterative approach under the designer's control;

7. the re-use of HEX between «compatible» process streams. This has already been taken into account here for H3/H4, and is not an issue for the other streams.

Considering the «cut-off» temperatures as additional improvements opportunities leads to the following results, presented on *Figure 2-14*:

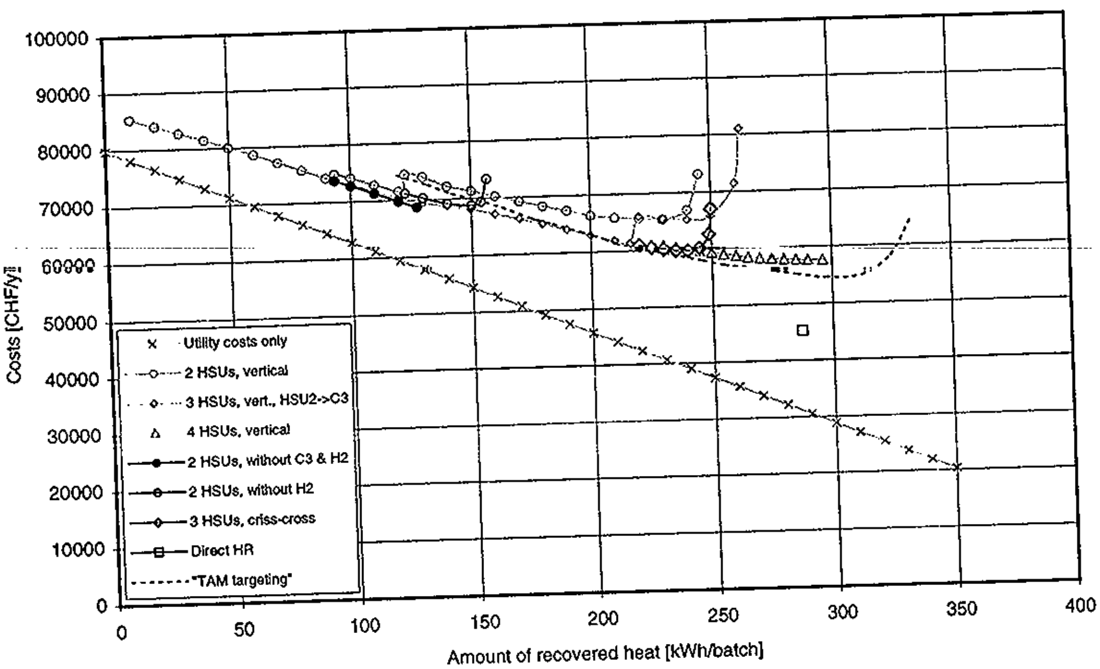


**Figure 2-14** Total annual costs of various heat integration solutions - example process EP1 (refer to text for further comments).

- with two HSUs, opportunities are readily identified as being related to the two step changes previously mentionned. First, H2 and C3 are removed from heat integration, allowing the HR to be increased up to 127.5 kWh/ batch (the heat content of C1) and TACs to be decreased by 7.7% compared to the same HR according to the vertical model. But since this solution integrates a limited set of process streams, it only provides an improvement of limited scope. The second opportunity is the exclusion of H2 alone (since the second step change is produced by H2, constraining HSU2). Again, this results in a local improvement of too limited scope to compete with the optimum HR (minimum TACs) found with vertical, two HSUs heat integration solutions. This demonstrates that although H2 is constraining the temperature of HSU2, it provides nevertheless a large opportunity for heat recovery within a low temperature difference, which is beneficial for heat integration;

- with three HSUs, a step change appears when H2 and C3 are vertically aligned, and H2 starts constraining HSU3 (if HSU2 is assigned to C3), or C3 starts constraining HSU1 (if HSU2 is assigned to H2). To allow for a further increase of the HR without such a constraint (i.e. increase HR beyond the step change), «criss-cross heat exchanges» can be used, as shown on *Figure 2-15*. The heat part from H2 which should normally be

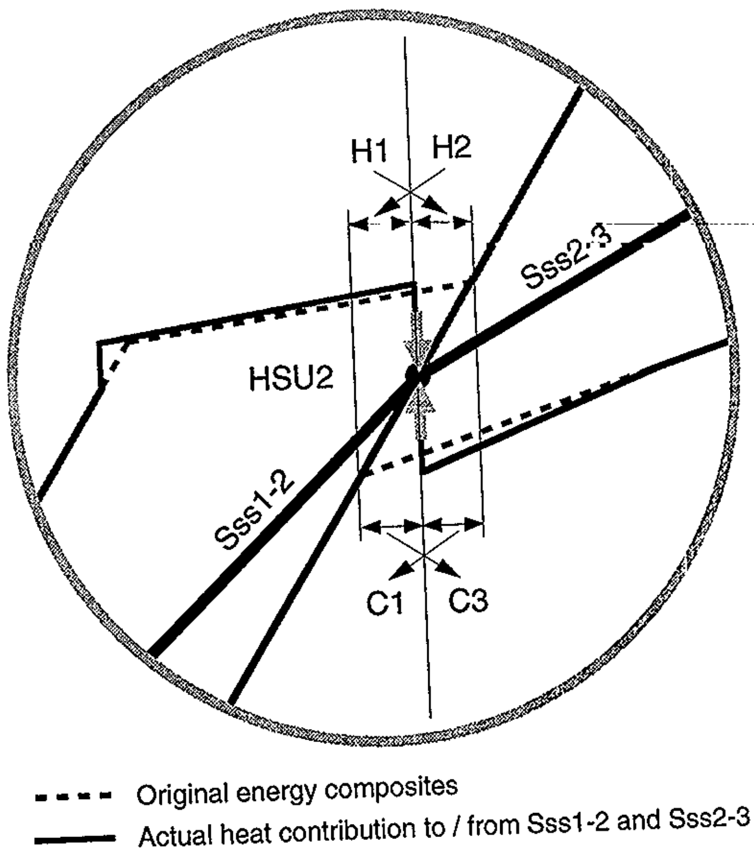


**Figure 2-15** Detail of criss-cross heat transfer «around» HSU2 to keep H2 in Sss1-2 and C3 in Sss2-3. The temperature of HSU2 is pinched between H1 and C1 temperature profiles - EP1 TAM composites, HR=250.2 kWh/batch.

supplied to Sss2-3 is feed in the Sss1-2, and replaced by an equivalent amount of heat from H1 which would normally be supplied to Sss1-2. Similarly, heat for C2 is fully supplied by Sss2-3, although part of it should come from Sss1-2 according to the vertical model; this is compensated by heat needed for C1 above 80°C which is now taken from Sss1-2. This strategy prevents both C3 from constraining HSU1, and H2 from constraining HSU3. However, the temperature margin of HSU2 decreases as the HR is increased, until an upper limit of HR=250.2 kWh/batch, for which HSU2 is fully pinched (as represented on *Figure 2-15*). Compared to 3 HSUs operating in standard «vertical mode», this allows the HR to be significantly increased while keeping the TACs at a level slightly below their minimum in vertical mode, until the pinch effect on the costs of the HEXs on H1 and C1 becomes prominent;

- with four HSUs, around the identified optimum, opportunities for criss-crossing do not exist. This is so because the limitation to a further increase of the HR results from the sudden temperature constraint introduced by C2 (the only remaining cold stream); none of the four HSUs is pinched before this point. Beyond this limit, using a fifth HSU is necessary (this is always so in the case of a vertical segment of composite: no criss-cross is ever possible). Resorting on criss-cross to further decrease the TACs is not sensible; since HSUs are assigned to C1, C2, H2 and H3/H4, only H1 could be criss-crossed (with H3/H4). But it does not make sense because H1 is not constraining;
- for comparison, the minimum TACs in direct heat integration (refer to Krummenacher & Favrat, 1995) is also represented on *Figure 2-14*. This is still 21% lower than the minimum TACs in indirect heat integration, for a similar degree of HR. Facing this apparently disappointing result for the indirect heat integration, one should recall the intrinsic high sensitivity of direct HENs to schedule variations. In addition, the cold streams and the hot streams of EP1 feature a relatively high degree of simultaneity (consider *Figure 2-9* on page 41), which is beneficial for direct heat exchanges but not common in batch processes;
- TACs calculated using a crude TACs targeting method are also reported on *Figure 2-14*. This targeting method assumes vertical heat transfer between TAM composites, and the assessment of capital costs is limited to HEXs, but excludes HSUs costs. However, to account for the need of heat transfer to (and from) intermediate storage streams, the heat transfer coefficient of the process streams is divided by a factor four, and further

multiplied by «duty ratio» factor equal to the duration of the stream over the batch cycle time. Although the calculation method is very crude, it provides in this case results of acceptable precision for the conceptual design stage. It intrinsically fails to provide structural information such as the required number of HSUs, or any related topological traps. The prominence, for EP1, of HEXs costs (20'400 CHF/y) compared to HSUs costs (7'800 CHF/y) partly explains the encouraging results of this crude targeting method. Improved ways of calculating the HEXs costs (accounting for the heat transfer coefficient of storage streams, etc.) and a simple calculation of the HSUs capacities and costs (accounting the simultaneity factor of streams, and possibly the minimum number of HSUs according to the procedure proposed in *Section 2.2.3* on page 27) should be developed. Defining a lower bound target to TACs would be a very valuable result. Validation of the targeting methods using a wider range of other processes is needed and should help in the definition of selection criterias.

This example deserves the following additional comments:

- except for the crude targeting, all other costs data are design data and not targeted data;
- the initial costs of both the HEXs and the HSUs are ignored (i.e. have a zero value). If an initial cost factor for HSUs was introduced, this would simply move the TACs points upwards accordingly, and penalize heat integration solutions with increasing number of HSUs;
- the area contributions of heat recovery matches (HEXs) on a same process stream are added before applying the cost function, which is a sound assumption. Data from practical projects is needed to further refine the cost function;
- the minimum number of HSUs both depends on the shape of composites curves (continuous variables) and the supply temperatures (the LSTPs, i.e. integer variables);
- the rather high simultaneity factor of streams is beneficial (with respect to the capital costs) to both the direct and the indirect heat integration modes. In the indirect mode, this results in required heat storage capacities often much lower then the heat actually transfered, as detailed calculations on EP1 have demonstrated;

- the number of HSUs and the storage pinches play a critical role in the search for the cost optimum heat integration and constrain the HR before the more fundamental process pinch comes into play. But depending on the shape of the composites, the process pinch may be the limiting pinch effect within a low number of HSUs;
- the mathematical properties of the model associated with the optimization of the operating temperature of the HSUs have not been analysed. Practical experience has shown that the Solver Tool (based on the Generalized Reduced Gradient (GRG) algorithm) is suitable to obtain the optimum solution, provided that the constraints (upper and lower temperatures bounds, and monotonic increase of the operating temperatures) are taken into account. Although not a formal proof, it has been observed that the same optimum solutions are obtained from very different initial feasible points.

#### 2.3.2.2 Proposed Procedure

A search for the optimum indirect heat integration of the process first described by Gremouti (1991) has made use of the same approach (Righetti, 1999). The sample of processes is of course too limited, and the processes of too limited complexity to validate the formerly described search strategy. But more complex processes can only be addressed in reasonable time if the most time-consuming tasks of setting up the problem description and defining the various costs contributions is automated. This is also a prerequisite for a systematic sensitivity analysis to be realized.

The search procedure towards a cost optimum heat integration scheme is heuristic, which rules derive from understanding the limitations (bottlenecks) to a further improvement of the heat recovery and a systematic use of the available degrees of freedom. It can be understood as a strategy to iteratively remove one bottleneck at a time. It remains to be verified on test cases of industrial relevance that the number of iterations and the systematic aspect of the search are manageable.

The procedure includes the following heuristic guidelines, organized in order of increasing «refinement» to first get an overview before going into more detailed calculations:

1. using the vertical model, calculate the TACs for various HR levels and for an increasing number of HSUs (start with 2). At first, all process streams

are taken into account in the TAM composites; the minimum number of HSUs and their feasible assignment range (temperature and heat margins) are defined using the procedure proposed in *Sub-section 2.2.3* on page 27. HSUs are attached to supply temperatures of streams within the identified range, accounting for the links between the assignment of adjacent HSUs (obviously present if the ranges overlap). If several streams start in the possible assignment range, the objective is to select the one which is the less constraining, i.e. the one which shall last be pinched as the HR is increased, while another assignment would pinch for smaller HR values. As a rule, avoid assigning HSUs to «small» streams, since these are likely to be removed or shifted to adjacent storage sub-systems. A sensible way to proceed is to first identify the largest HR values (in vertical mode) which can be achieved with two HSUs, three HSUs, four HSUs, etc., and the related assignement range. Then assign the HSUs to streams which allow to best balance the available TDFs. This strategy assumes (as observed for EP1) that the minimum TACs are to be found quite close to the upper limit of HR for a given number of HSUs, and hence the assignment of HSUs has to be decided consequently. Note that the «right» assignment of an HSU is not an independent property, but it is a global issue interrelated with the other adjacent HSUs. This guideline might need further refinement based on experience and analysis of more cases;

2. the TACs calculations are performed for various HR values, and in particular close to each major change which is associated with a change of the stream population within each storage sub-system. These major changes are «registred» as opportunities for further improvements to be analysed later. In the vertical model, these changes potentially result in a step change of TACs because of a step change of one HSU temperature;
3. if several configurations exist for assigning the HSUs, assess these using the same procedure;
4. the time has come for giving up the vertical simplified model and embarking on shifting of streams between Sss and using criss-crossing to maintain heat balance if need be, so as to improve the economics (for the same level of HR) or improve the HR (at similar or lower TACs). The basic principle consists in identifying the bottlenecks and making use of the action most likely suited to remove them (or delay their effect). Bottlenecks are most generally related to the supply temperature of the streams integrated in a storage sub-system; at defined HR values (in vertical mode), the temperature margin of a HSU undergoes step

reductions, or even becomes infeasible, requiring a new HSU to be introduced. One can distinguish various typical cases (e.g. depending on whether the HSU is subject to a single-side constraint (hot or cold), or rather a double-side constraint (although one can be more critical), or depending on whether the constraining stream is of the same type as the stream the HSU is assigned to, or of the opposite type). Actions to remove a HSU related bottleneck include shifting of cold constraining streams to adjacent (above, right) Sss, shifting of hot constraining streams to adjacent (below, left) Sss. Criss-cross heat exchanges are used around the crossing of a constraining hot and constraining cold stream, that would otherwise requires an additional HSU to be introduced (e.g. refer to the case of C3 and H2 at the origin of the criss-cross represented on figure *Figure 2-15* on page 56). Always remove the most constraining stream at a time (e.g. for the supply temperature, if, within a Sss, the cold stream with the second highest supply temperature is removed (shifted) instead of the one with the highest, there will be no debottlencking effect at all). As already mentionned, the discrete effects related to the number of HSUs and the supply temperature of streams are prevailing over the effect of process pinch, which seldom comes into play for the global optimum. Using this principle, systematically explore the various opportunities.

5. finally, for the best performing configurations, search for further opportunities to improve the cost efficiency by considering possible shifting or removing of unconstraining small streams (if they were constraining, they would have already been shifted). Just like for continuous processes, small streams are associated with cost penalties. A low heat transfer coefficient and/or a small duration make this even worse. The obvious search strategy consists in shifting these cold streams to higher Sss (hot streams to lower Sss), or even remove them from heat integration. If streams of significant heat content but low heat transfer coefficient and/or low duration are present, it is expected, unlike the EP1 test case, that the optimum (minimum) is located significantly before an upper limit to HR is encountered. Therefore, around the minimum, HSUs are provided with enough temperature margin so as to try shifting these streams (totally or in part, if the supply temperature is not constraining). The effect of the schedule of streams on the HSU capacities should also be taken into account while assessing which streams are candidates for shifting; this shall likely be relevant only for large HSU to HEX capital costs ratios.

### 2.3.2.3
### *Comments*

As already mentionned, experience is still lacking to validate this strategy, which has the advantage of providing insight in the major trade-off effects, but the drawback of combinatorial complexity without the guarantee to reach the optimum. Additional cases studies shall help getting a quantitative assessment of the relative significances of the various effects and translating this experience into guidelines.

The heuristics nature of the procedure does not guarantee that the optimal solution is identified; the use of the procedure for processes including about 20 streams should demonstrate whether the associated combinatorial difficulty is manageable or whether user insight and decisions are needed to further restrict the search space. The degree of freedom likely to be responsible for the introduction of the largest combinatorial difficulty is the selection the optimal criss-cross heat exchanges; a method inspired by the diverse pinch concept (Rev & Fonyo, 1991) has been identified as partial solution to this problem, but remains to be developed.

## 2.3.3
## Stochastic Optimization Using Genetic Algorithms

The heuristic method provides insight in the major trade-off effects linked to the integer decisions, but cannot efficiently address the fine tuning of continuous variables. Therefore there is an obvious need to address this optimization problem using a GA based approach. The working principle of GAs is introduced in Sub-section 3.3.2 on page 94.

Refering to the mathematical model formerly described in *Sub-section 2.3.1* on page 44, the major issues with respect to a GA based optimization are concerned with:

- the choice of the independent variables;
- the encoding of these variables;
- and the possible decomposition into several optimization levels.

From the mathematical formulation, the following particularities can be highlighted:

- independent variables are of two categories: the operating temperature of the HSUs ($T_k$), and the HEX related variables ($Q_{i,k}$, $Q_{k,j}$; or $T_{i,k}$, $T_{j,k}$; or $A_{i,k}$, $A_{j,k}$; etc.);
- the potential number of feasible HEXs on a process stream $p$ depends on the operating temperature $T_k$ of the HSUs (and of course of its supply $T_{S,p}$ and target $T_{T,p}$ temperatures, but these are part of the problem data and are not independent variables adjusted during optimization). E.g., if the temperatures of HSU1 and HSU2 are lower than the supply temperature of a cold stream $T_{S,j}$, than HEXs between this stream and the storage sub-systems Sss1 and Sss2 are infeasible, and $T_{j,2} = T_{j,1} = T_{S,j}$ (refer to *Figure 2-12* on page 46). Hence, the operating temperatures of HSUs have major structural consequences for the definition of feasible HENs;
- as implied by the positive temperature driving force constraints (*Equations 2-4 to 2-9*), the lower boundary on $T_{j,k}$ is defined by the value of $T_{j,k-1}$; the same dependency can be seen from *Equation 2-1* to account for the monotonic increase of the temperature of HSUs. But the GA is not able to account for this dependency of bounds on other independent variables of the problem. Improper specification of the bounds on each variable goes with the risk for the GA to generate (by cross-over, or mutation, etc.) infeasible values, i.e. values that lay outside the feasible boundaries. These GA generated solutions (individuals) should first be checked, and then, if not feasible, either rejected, penalized, or corrected to make them feasible, which in any case spend valuable computing time. An alternate solution is to select other independent variables characterized by fixed boundaries.

### 2.3.3.1 Independant Variables and Encoding for the GA

Taking the former comments into account, the independent variables are as follows:

- for HSUs: operating temperature $T_k$. But the GA shall operate on reduced, dimensionless variables $X_k$ expressed in the following way:

$$X_k = \frac{T_k - T_{k-1}}{T_{max} - T_{k-1}} \quad \text{with} \quad 0 < X_k < 1 \tag{2-13}$$

using this definition, the upper and lower bounds on $X_k$ are fixed, irrespective of the value of the independent variables (it is the meaning of

$X_k$ in term of $T_k$ which changes as function of other variables). These $X_k$ variables will be decoded in the model, starting from $T_1$ to $T_{kmax}$, to take the propagation of constraints into account; $T_{max}$ is the maximum feasible operating temperature of an HSU, which is limited by either the storage fluid or the hot end of composite curves.

- for HEXs: intermediate stream temperatures $T_{i,k}$, $T_{j,k}$. But the GA shall manipulate the following reduced, dimensionless variables $X_{i,k}$ (for the case of hot process streams) expressed as:

$$X_{i,k} = \frac{T_{i,k} - T_k}{T_{i,k+1} - T_k} \quad \text{with} \quad 0 < X_{i,k} < 1 \quad \text{(for the hot streams)} \qquad \text{(2-14)}$$

  with this encoding, the upper and lower bounds on $X_{i,k}$ are fixed, irrespective of the value of the independent variables (it is the meaning of $X_{i,k}$ in term of $T_{i,k}$ which changes as function of other variables). These $X_{i,k}$ variables will be decoded back in the model, starting from $T_{i,k_{max}-1}$ towards $T_{i,1}$, to take the propagation of constraints into account. Cold stream variables are encoded in a similar way.

Encoding, decoding, and uniform boundaries are likely less CPU time consuming than checking and correcting/eliminating unfeasible solutions. Constraints of monotonically increasing temperature of HSUs and positive temperature driving forces are automatically satisfied by the above definitions, and the model reduces to simple, straighforward calculations.

Note that the variables to be manipulated by the GA could alternatively be defined as:

- for HSUs: $T_1$, then $\Delta T_{2,1}$, $\Delta T_{3,2}$, $\Delta T_{4,3}$, etc.;
- for HEXs: the heat exchanges $Q_{i,k}$ could be specified by the area $A_{i,k}$ of the associated HEXs, which in any case leads to feasible solutions (with $0 \le A_{i,k} < \infty$). This choice is plagued with the need to iteratively solve for the $T_{i,k}$, because of the non-explicit relationship between $A_{i,k}$ and $T_{i,k}$.

This confirms the critical role played by the choice of independent variables for the efficiency of the optimization model.

### 2.3.3.2
### Optimization on Two Levels

Noting the essential structural influence of the $T_k$ variables, a decomposition of the optimization into two levels becomes an obvious strategy. This choice is backed by the following additional considerations:

- with a single level optimization, any solution (individual) includes both HSU and HEX variables. The population of solutions evolves through reproduction, blend cross-over and mutation. It is hoped that good features of the parents be «cumulated» by blend cross-over. But what happens when cross-over is performed between individuals which do not feature the same structure, i.e. not the same number of HEXs, originating in different $T_k$ values. The offspring will probably be unfeasible, i.e. be a so-called «monster». The solution to this problem generally relies on the concept of distance (refer to Olsommer, 1998, pages 135-136). An alternate way to go is the optimization on two levels;
- compared to other engineering optimization problems, the problem at hand features a significantly lower complexity level. The methodological benefit of choosing an optimization on two levels should unlikely be payed by excessive computing time.

The optimization procedure using two levels is sketched on *Figure 2-16*. Note however that an external loop on the number of HSUs (starting with $K = 2$) should be added to get an overall optimization, since the optimization procedure of *Figure 2-16* assumes a given number of HSUs, specified by the user.

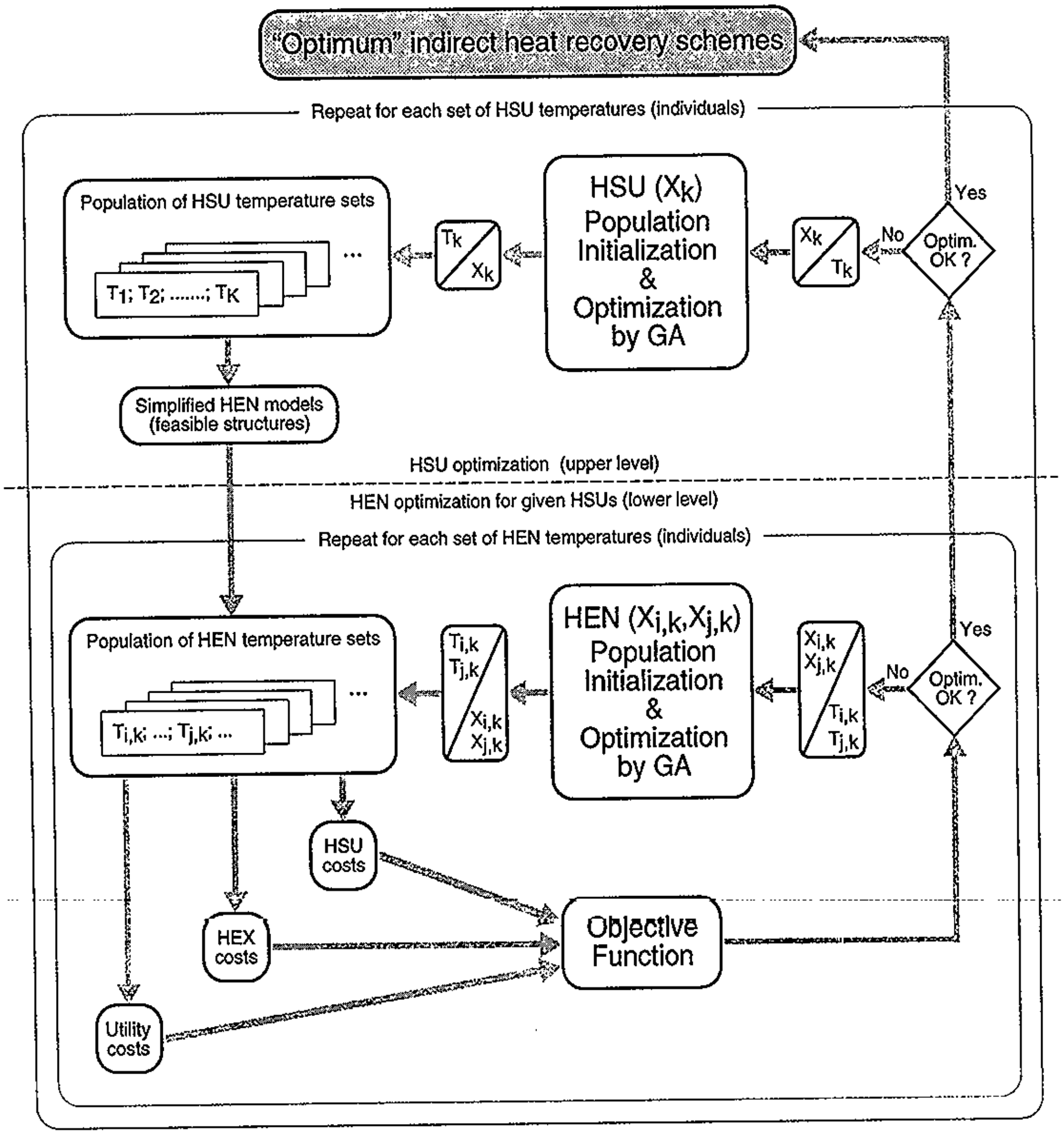


**Figure 2-16** Principle of a two-level, GA based solution approach to the design and optimization of 100% indirect heat recovery schemes.

### 2.3.3.3 Heat Balance Constraints

In the mathematical formulation, constraints given as *Equation 2-2* on page 48 require each storage sub-systems (Sss) to be balanced over a batch cycle time (heat or mass balance). Each heat balance constraint associated with each Sss reduces the number of independent variables (representing the individual heat contributions to/from Sss) by one unit. But most of the time, the set of $T_{i,k}$ and $T_{j,k}$ generated by the GA shall not allow to satisfy these constraints, i.e. these solutions would not be feasible and should be penalized. This approach has the additional drawback of neither allowing utilities to be supplied to process streams through (intermediate) Sss, nor allowing intermediate, lower costs utilities for utility requirement at lower exergy levels.

To avoid the above difficulties, the heat balance constraints (achieved exclusively by process streams) can be relaxed, and the heat balance be achieved by external utilities. Taking the costs of these utilities into account, the optimization algorithm shall progress towards minimizing their usage and hence automatically achieving the heat balance exclusively with process streams - if this minimizes the objective function. This approach is more general than the one requiring strict heat balance at the onset.

#### 2.3.3.4 Possible Extensions of the Model

The following extensions of the above GA based approach could be considered later:

- the re-use of HEX units. Since the design of indirect HR schemes is basically independent of the time slices, the only re-use mode to be considered is the repipe of HEXs units for streams which do not overlap in time;
- the opportunity to take full account of the hot process water requirements to avoid related storage-to-cold process streams HEXs;
- the opportunity to reduce the number of HSUs by considering the slice-wise related supply temperatures, which allow to ignore the supply temperatures of process streams which are «included» (both in time and in temperature) into other process streams. This goes with increased complexity of the HEN structure, since HEX units are no more strictly in parallel on the storage side, replaced by a serial-parallel HEN structure;
- and finally, the extension to mixed direct-indirect HR schemes, under the the simplifying assumption of exclusive direct matches.

## 2.4 Mixed Direct-Indirect HR Schemes

### 2.4.1 Introduction

Mixed direct-indirect heat recovery is thought here as an extension of the indirect mode towards more cost efficient heat recovery schemes without sacrifiying the flexibility of the process. Direct matches are therefore more an exception than a rule, restricted to cases which improve the cost-effectiveness of the heat integration without sacrifying its flexibility. In the context of a Pinch Analysis approch, these opportunities are identified using heuristics rules. Very first trials have resulted in a few guidelines.

## 2.4.2
## Guidelines to Identify Potential Direct Matches

Direct matches should decrease the capital costs (both HEX and HSU costs) without adding significant complexity or operability problem to the HR scheme. Direct matches shall rather be «one-to-one» matches, at any given time (unless the matched streams are part of the same master/slave group of streams, which corresponds to a semi-continuous sub-processes). The following guidelines for identifying potential direct heat recovery matches can be drawn:

- ♦ obvious preliminary conditions are feasible temperature driving forces and overlapping time schedule;
- ♦ a significant amount of heat recovery (when compared to the 100% indirect HR) should be possible;
- ♦ potential candidates for a beneficial direct heat recovery are streams which are either constraining a HSU (particularly if the cost of HSUs is relatively high) or have a relatively low heat transfer film coefficient, for which a "suitable" stream of opposite type can be found. A "suitable" stream means that the temperature driving forces of the match are smaller or equal to that on the TAM composites (otherwise the cost-efficincy of the indirect heat recovery is penalized);
- ♦ the stream matches for which one of the streams is completely included both in time (with sufficient margin) and temperature are good candidates for direct matches.

A more systematic way to go is to apply the OV to determine the best set of exclusive matches, from which some matches may be left if they are sensitive to schedule variations. But selecting a reasonable value for $\Delta T_{min}$ between matched streams remains an unaddressed issue.

To bypass the problem, heat rate and match information could be derived from MBC supertargeting (starting from slice-wise HENs generated according to the MBC pinch design method would not make sense, because of the time needed to generate such HENs by hand).

### 2.4.3 Independent Variables for Optimization

The optimization variables are chosen to be:

- the overall heat recovery;
- and the $\Delta T_{min}$ of individual matches.

Note that chosing the match-wise heat recovery instead of match-wise $\Delta T_{min}$ is not sensible because of frequent "threshold" matches (defined by analogy with threshold processes).

### 2.4.4 Example

The above guidelines have been applied to the EP1 example process (refer to *Figure 2-1* on page 18). Direct matches H1-C1 and H2-C3 have been selected, while the remaining parts of the streams which could be integrated were taken into account in the indirect TAM composites. Stream H2 (which features a larger MCp compared to C3) is splitted to recover heat at a valuable temperature level for indirect HR. Using a parallel rather than a serial configuration not only allows the heat to be recoved at a useful level, but also increases the temperature driving forces (TDFs) in indirect HR, which are most critical, at the expense of reducing the TDFs available for direct HR.

The minimum TACs have been searched for with 2, 3 and 4 HSUs, assuming a vertical definition of each storage sub-system. The minimum costs solution is found to be 13% more expensive than the direct HR, and 11% cheaper than the 100% indirect HR (with $\Delta T_{minH1\text{-}C1}$=10°C, $\Delta T_{minH2\text{-}C3}$=2°C, and overall HR=310 kWh/batch, of which 65% is transfered by the direct matches).

The optimization has been performed by trial and error. Unlike the case of 100% indirect HR, the mixed mode is really difficult to optimize. The shapes of TAM composites for indirect heat recovery are changed each time the match-wise $\Delta T_{min}$ are adjusted, requiring repetive changes to the assignment of HSUs to be made. Complex trade-off effects are observed.

This simple trial confirms that the optimization of mixed direct-indirect heat recovery can only be addressed by automated synthesis methods. Nevertheless its provides with some useful insight, e.g. with respect to the type of simple mixed direct-indirect HEN configurations to be taken into account in an automated synthesis approach.

## 2.5 Schedule Effects and Rescheduling

Rescheduling is an additional degree of freedom in the overall optimization of batch processes. A simultaneous optimization of both the schedule and the indirect HR scheme could be desirable, but would very likely be impracticable. A more reasonable approach is to first optimize the HR scheme (keeping the schedule unchanged), and then question the schedule so as to determine whether a rescheduling of streams could improve the solution.

In pratice, only few streams can actually be rescheduled with respect to other streams. In a Pinch Analysis perspective, a graphical representation providing the designer with global insight in the problem is highly desirable.

Inspired by the split GCC (refer to Kemp, 1991), used to assess the integration of a new equipment into an existing process («background process»), a new graphical tool is proposed to readily assess the potential for reducing the capacity of a HSU by rescheduling a stream (or a master/slave group), as illustrated on *Figure 2-17*.

Assume a HSU to which heat is supplied by streams H1 and H2, and from which heat is removed by streams C1 and C2:

- the cumulated, individual heat contributions, as well as the overall cumulated heat (of course, balanced on the batch cycle) are represented on *Figure 2-17*, «Base case schedule»;
- «Rescheduling C2» represents the case where contributions of H1, H2 and C1 are grouped together (i.e. all heat contributions but C2), while the one of C2 is represented separately (and actually «mirrored»). In this representation, the maximum required heat capacity is measured (vertically) between the H1+H2+C1 curve and the C2 curve, i.e. the C2 curve has replaced the horizontal baseline. Four ways of rescheduling C2

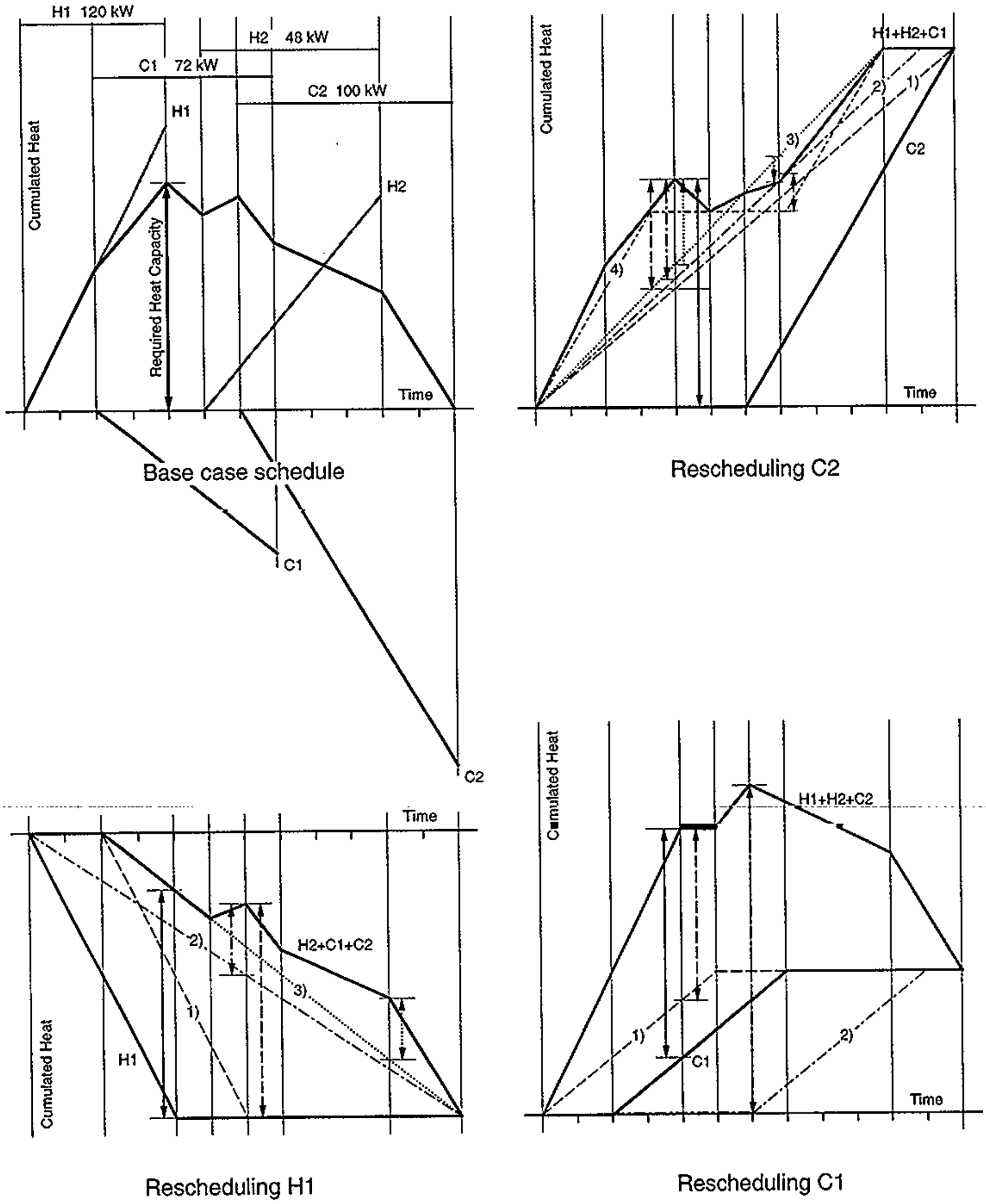


**Figure 2-17** Assessing rescheduling opportunities (see comments in text).

are considered (note that if the mass flowrate had to be kept unchanged, the reduction potentiel would be very low):

1. C2 starts earlier, while the finish time is unchanged (in this case C2 is like a continuous stream, since it extends over the whole cycle time). The maximum heat inventory still appears at the same time, but is reduced by a factor of about 2;

2. C2 starts earlier and finishes earlier, so that the maximum heat inventory is slighlty reduced compared to case 1;
3. if C2 starts at the same time as in cases 1 and 2, but finishes earlier, the maximum heat inventory increases again compared to case 2, since the inventory is defined as the difference between the largest positive value and the «largest» negative value;
4. in the particular case where C2 does not require to be heated at constant rate in one run and can be splitted in time in several sub-parts (e.g. an uncritical feed could be preheated in part and wait in the reactor), the capacity of the HSU could be reduced to a large extend. This case can be seen as optimizing the use of the available storage capacities of process equipments in complement to HSUs;

- «Rescheduling H1» assesses the potential of decreasing the storage capacity by rescheduling H1. The potential is large for rescheduling scenarios 2) and 3), both assuming the finish time is delayed until the end of the batch cycle (maximum possible delay). If the flowrate has to be kept unchanged (case 1), the reduction potential is very limited.
- «Rescheduling C1» demonstrates that the potential is quite limited when the mass flowrate has to be kept unchanged. In addition, two interesting effects (insensitivity margin and sensitivity effect, respectively) can be seen:

1. whenever C1 finishes earlier than the time of the maximum of the H1+H2+C2 curve, any further advance or change of the mass flowrate shall not reduce the required heat storage capacity;
2. symetrically, if C1 finishes after this time, any further delay on start of C1 increases the required capacity.

Of course, practical constraints (mainly from recipe and use of equipments) shall determine which rescheduling, and to which extend, are actually feasible; *Figure 2-17* assumes no limitation for demonstration purpose, but this is never the case !

This representation can be seen as a simple evolution of the representation given in Sadr-Kazemi & Polley (1996) and the time composites developed by Wang & Smith (1995) for time pinch analysis.

The proposed representation is actually suited for analysing the potential to decrease the storage capacity of either an «isolated» storage sub-system (i.e.

two HSUs working out of phase) or of a single HSU in the «chain» of HSUs. But in the later case (when the storage sub-system is not isolated), or when the stream to be rescheduled is supplying to or sinking heat from several sub-systems, one has to simultaneously account for the effect of rescheduling on every related HSUs, which makes the analysis less trivial. Assessing the rescheduling of several, not related streams simultaneously is not straightforward either.

The representation could also be used to gain insight and assess the sensitivity of required storage capacity to variations of the schedule of any streams. But a systematic methodology to modelize the likely variations of schedule remains to be developed.

## 2.6 Summary

The relevance of the indirect mode of heat integration for flexible batch processes has motivated a detailed analysis of various issues and the development of two complementary design methodologies - a heuristic Pinch Analysis based strategy and an automated, GA based design and optimization approach. Further work is needed to validate these methodologies and provide reference data, against which simple targeting methods should be developed.

As part of the heuristic strategy:

- the degrees of freedom available for optimization are described;
- a systematic method is proposed for the determination of the minimum number of HSUs for any feasible HR value. The method is based on the TAM composites on which "limiting supply temperature profiles" (LSTPs) are added. The representation helps in assigning the HSUs and provides the user with insight in the problem;
- the concept of storage pinch is analysed to understand why values as low as 1-2°C are found in costs optimum solutions;
- the minimum number of HSUs (determined assuming vertically defined storage sub-systems) can sometimes be reduced when considering the slice-wise (instead of the stream-wise) supply temperatures. This opportunitity is plagued by the need to verify the feasibility of heat transfer and by structurally more complex HENs;

- the indirect heat integration of a simple example process is described in details. It exemplifies the strategy and demontrates the key role of the supply temperature of streams, the effect of the storage pinch on the objective function and possible ways to remove one bottleneck at a time. The heuristic strategy is suitable for integer decisions, but cannot efficiently address the fine optimization of continuous variables such as the heat contribution of each process stream to / from each storage sub-system;
- guidelines to extend the heuristic strategy to mixed direct-indirect heat integration are listed, along with preliminary results.

With respect to the automated synthesis approach:

- the mathematical model of the problem as well as the independent variables and the set of constraints are described;
- a GA based optimization approach is presented. The approach includes two levels, the upper level being concerned with the optimization of the operating temperature of HSUs, while the heat rate of HEXs are optimized at the lower level (the HEN structure being inherited from the upper level). A special coding scheme of the independent variables is proposed to prevent the GA from generating infeasible solutions.

A simple graphical representation allowing for an easy assessment of rescheduling opportunities is introduced.

# Chapter 3

# AUTOMATED BATCH HEN DESIGN

## 3.1 Introduction

### 3.1.1 Motivation

*Chapter 2* has focused on indirect heat recovery because of the significance of this robust mode of heat integration for flexible batch processes. Direct batch HENs are still of importance and their automated design has to be addressed, at least for subsets of streams (subsets of time slices, respectively) featuring robust scheduling, i.e. for which HEXs to be placed are reasonably insensitive to the likely schedule variations. To this aim, a method to measure or specify the likely schedule variations remains to be developed, although significant related work on operation and control strategies of batch processes has already been achieved (e.g. Klemes *et al.*, 1994). In particular, delay compensation strategies have been proposed. With respect to heat integration, unlike the common "zero-wait operation mode" (in which the start of the batch is calculated so that the product(s) can be transfered to other units without any idle time (in the base case schedule, i.e. in the absence of any perturbation)), a "systematic idle time mode" could help to synchronise matched streams (in this mode, batches are started as soon as possible, so that idle time is available at the end of each stage (except the bottleneck stage) to cope with delays without effect on the critical path). The delay compensation is possible (within given idle time limits) for streams which are neither on the critical path nor related to critical tasks, e.g. biological reactions, for which very precise time-temperature profiles are prescribed for yield and quality reasons.

The design of optimal batch HENs has been recognized as a non-trivial task. Designing batch HENs "by hand" using MBC design heuristics is time-consuming and requires skills and experience (Krummenacher & Favrat, 1995). Methods for automated design of batch HENs using a combinatorial approach suffers from limitations imposed by the related simplifying assumptions (Hellwig & Thöne, 1994; Uhlenbruck, 1995).

Automated methods for designing batch HENs should also be able to account for various practical constraints with respect to the feasibility of matches.

The main issues of the design of batch HENs are analysed, and a solution approach, based on genetic algorithms, is proposed. The practical implementation and testing remain to be achieved. Early conclusions with respect to some important issues, such as the computational complexity and time requirements, can't be drawn at this stage.

An in-depth review of relevant litterature can be found in *Section A.4* on page A-26, and *Section A.5* on page A-34.

### 3.1.2 Main Issues

Compared to continuous HENs, batch HENs are characterized by:

- fewer HEXs units, hence generally a less complex overall HEN structure;
- an increased design complexity arising from the need to account for the feasibility of the HEN with respect to each time slice;
- the possible re-use of HEX units across time slices in various ways, giving rise to increased combinatorial complexity;
- more complex interconnections (piping, valves and by-passes) required to cope with the re-use of HEX units and the HEN being"tailored" to each time slice.

As described by Jones (1991), three major ways of re-using HEX units have to be considered:

- conventional, in which the HEN remains structurally unchanged, i.e. HEX remains between the same streams, and in the same sequence with respect to other matches. HEX units are re-used across time slices by pairs of streams extending over more than one time slice;

- resequence, in which case the HEX units remain between the same streams, but their sequence may be changed from one time slice to the next;
- repipe, in which HEX units can be "repiped", so as to operate between any other pair of streams.

Re-using a HEX unit in any of the three modes generally means re-using only part of its design area, which requires by-passing part of flowrate (on either sides) to reduce the active area by reducing the log.arithmic mean temperature difference.

By-passes are therefore required for any of the three re-use modes. More complex and potentially costly valving and piping are required for resequence and repipe. HEX units generally need cleaning before being repiped.

Streams flowing in the same pipe/same equipment (same location) at different times represent another case of HEX re-use, somewhat similar to repipe.

Generating and evaluating all possible repiped and resequenced HEN structures from a basic "masterstructure" would be complex and time-consuming. Fortunately enough, various practical constraints generally restrict the number of repipe and / or resequence opportunities.

### 3.1.3 Introducing an Example Process

The following process, described by its stream list (*Table 3-1*) and Gantt diagram (*Figure 3-1*), is used throughout this chapter to illustrate the various concepts. Temperature or flowrate information is not included in the stream list, since this is actually not needed for the purpose of the presentation. In addition, in order to exemplify various cases using one single process, the example process had to be devised and is not an actual process. The constraints restricting repipe and resequence opportunities are more difficult to justify since they cannot be related to actual equipments and fluids properties.

| Stream Name | Fluid & Properties | t start 1) [min] | t stop 1) [min] | Location |
|---|---|---|---|---|
| H1 | fluid A, liquid, low viscosity, high density | 640 | 300 | 1 |
| H2 | fluid A, liquid, low viscosity, high density | 420 | 620 | 1 |
| H3 | fluid B, liquid, high viscosity, middle density | 90 | 340 | 2 |
| H4 | contaminated waste fluid C, gas (heat recov.) | 300 | 640 | 3 |
| H5 | contaminated waste fluid A, liquid, (heat recov.) | 300 | 540 | 4 |
| C1 | fluid D, liquid, low viscosity, high density | 150 | 300 | 5 |
| C2 | fluid D, liquid, high pressure, high temperature | 150 | 620 | 6 |
| C3 | fluid C, gas | 640 | 300 | 7 |
| C4 | fluid B+water, liquid, high visc., middle density | 420 | 620 | 8 |
| C5 | fluid F in evaporation | 150 | 540 | 9 |

Notes: 1) Batch cycle: 0 - 720 minutes

**Table 3-1** Stream list of example process EP2.

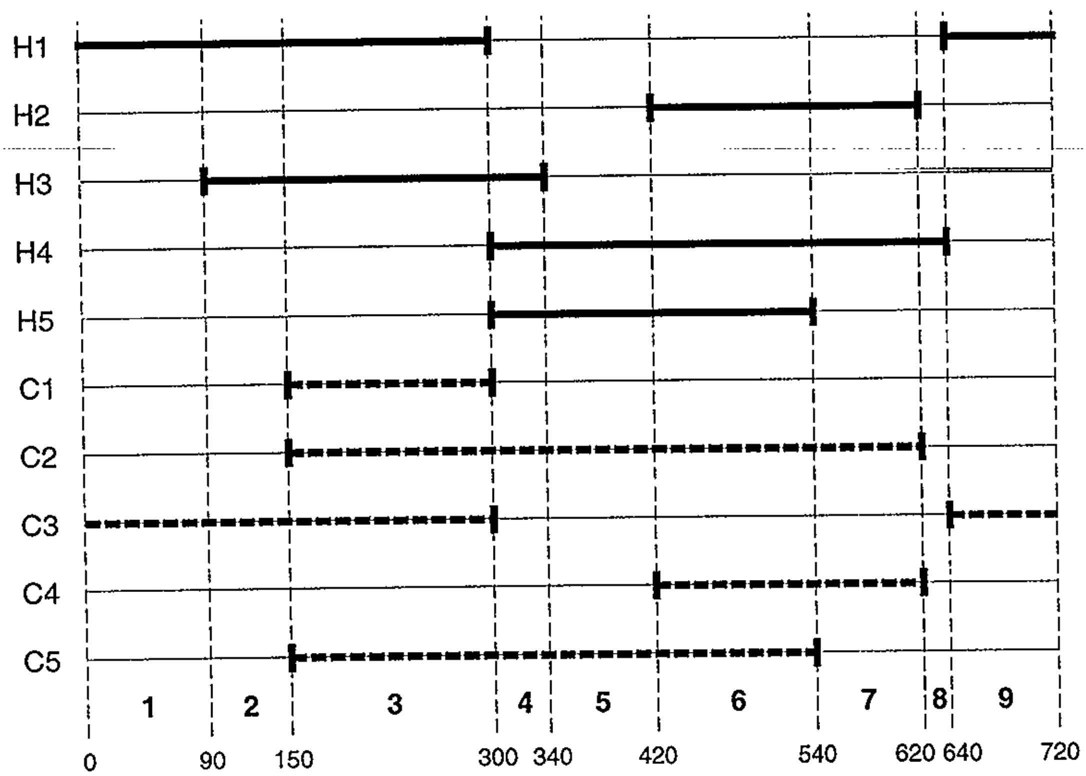


**Figure 3-1** Gantt Diagram of example process EP2.

### 3.1.4 Organization of the Chapter

*Section 3.2, "Constraints on the Re-use of HEX Units"*, on page 80, describes the various types of constraints restricting the repipe and the resequence of HEX units between time slices. A simple methodology is proposed to categorize into:

- the need for similar thermo-physical stream properties (*Sub-section 3.2.2*);
- the chemical compatibility and related cleaning requirements (*Sub-section 3.2.3*);
- the limitations imposed by the process time schedule on repipe (*Sub-section 3.2.4*) and on resequence (*Sub-section 3.2.5*).

In addition, *Sub-section 3.2.6* demonstrates how a by-pass allows a given HEX area to be decreased to suit a case with smaller area requirement.

*Section 3.3, "Proposed Solution Approach Based on Genetic Algorithms"*, on page 92, presents the main issues in design & optimization of HENs and discusses the choice of the solution approach (*Section 3.3.1*). The working principle of Genetic Algorithms (GAs) is recalled (*Section 3.3.2*). *Sub-section 3.3.3* describes in more details the solution approach and its decomposition into an upper level, where the structure of the overall HEN (the masterstructure), as well as the area values, are optimized, and a lower level which optimizes the use of the given HEX units for each time slice, in terms of both structure and actual HEX areas. Related assumptions are highlighted in *Section 3.3.4*, while *Section 3.3.5* focuses on the way the masterstructure can be encoded for use by a GA. The search for minimum utility costs, given the (maximum) area of HEX units, is addressed in *Section 3.3.6*.

In *Section 3.4* on page 110, guidelines are presented which allow to reduce the number of time slices to consider at both the MBC supertargeting stage and the GA automated design stage.

*Section 3.5* summarizes the chapter and highlights the need for further work.

# 3.2 Constraints on the Re-use of HEX Units

## 3.2.1 Introduction

As previously mentionned, Jones (1991) considered three different ways of re-using HEX units for Multiple Base Case (MBC) design of continuous processes: conventionnal, resequence, and repipe. However, guidelines for selecting the appropriate mode of re-using HEX units have not been presented. In addition, the MBC supertargeting algorithms proposed by Jones do not allow for mixed mode of HEX re-use, e.g. critical streams requiring conventionnal, while others would tolerate resequence and/or repipe. Separate MBC supertargeting algorithms have been developed for either repipe, or resequence, or conventionnal; mixed mode of HEX re-use could be considered during design, if needed.

The ability to simultaneously account for the various modes of re-using HEX units is of utmost importance in the perspective of automated batch HEN design. In order to avoid impractical HEN structures (and useless calculations), cases where repipe is out of question should be identified at the onset.

The repipe opportunities are restricted by three types of constraints:

1. the compatibility of thermo-physical properties of the streams;
2. the chemical compatibility of the streams;
3. operational constraints resulting from the time schedule of the streams.

Constraints 1. and 3. also restrict the opportunities for resequence.

## 3.2.2 Thermo-physical compatibility

Different heat exchanger types (e.g. shell-&-tube, plate, coaxial double tube, faling film evaporator, high temperature gas recuperator, etc.) each have their specific application range and their recommended operating conditions.

For example, plate heat exchangers are neither suitable for high viscosity liquids nor for gases; their maximum operating temperature is imposed by gasket material, while their mechanical design principle restricts the maximum allowable operating pressure, as well as the pressure difference between the primary and secondary sides. In a repipe perspective (i.e. operating an HEX unit with another stream on one side - or between another pair of streams), such constraints have to be taken into account. A plate HEX designed for heat recovery from low temperature liquids cannot be repiped into a high temperature gas recuperator !

Constraints on operating conditions (which determine to a large extend the type of HEX to be used) can generally be formalized in terms of:

- the temperature span of a stream;
- the operating pressure;
- the phase (solid, liquid, gas).

The repipe of an HEX also requires that the pressure drop across the unit do not be too different, that is, the pumping power remains acceptable. Detailled expressions of the pressure drop are complex and depend on the HEX type; however, among other factors, the following properties are of particular relevance:

- the viscosity of the stream;
- the density (or specific volume).

Based on the constraints, and the related properties mentionned above (the list of which might not necessarily be exhaustive), the idea is to divide up the streams into separate groups of "thermo-physical" compatibility.

Streams within a group of "thermo-physical" compatibility feature similar enough properties that they could potentially use the same HEX (at different times). This concept of compatibility is not a binary property, i.e. there is no absolute criteria that allows unambiguous decision about the compatibility. The concept is rather fuzzy. The degree of similarity to which streams properties / operating conditions are to be considered as compatible is up to the designer, knowing that strong (strict) compatibility constraints will lead to safe designs, but with the potential drawback of not being economically optimal since HEX units might not be used as much as possible. The concept of compability is somewhat like a control parameter for trading-off safety against cost efficiency of the design.

Identifying the "thermo-physical" compatibility groups isn't an obvious task; experience and insight are needed. Streams properties have to be compared, but it would also require that likely matches and suitable HEX types be thought of, since the operating range and the related compatibility conditions depend on the type of HEX.

No guidelines are listed here; many of these could be derived from "best engineering practice" and, to a large extent, be automated as "expert-system rules".

As described later in this chapter, the re-use of HEXs across time slices (be it by conventional, resequence or repipe) generally requires the active area to be reduced using a by-pass. Since optimized design of HEXs are often operated not so far from the laminar mode, limited decreases of the flowrate may lead to large adverse effect on the film coefficient. But this effect can hardly be anticipated at the onset and has to be verified after optimal HEN structures have been identified. Within the number of good structures, there shall hopefully be structures that do not feature such problems. In the opposite case, the compatibility groups should be re-evaluated so as to avoid these problems. Alternatively, HEXs units can be designed as a serial arrangement of sub-units individualy tailored to the various area requirements.

Note the following simple practical rules and comments:

- compatibility groups featuring less than two streams are not of interest;
- phase changes in segmented streams should be given due consideration: a software programme should actually "split" the segmented stream into as many separate streams as the number of different phases (needed for both repipe and resequence opportunities);
- a compatibility group can include both hot and cold streams;
- compatibility should also be checked for utility and storage streams ... but the implications remain to be further analysed.

#### *3.2.2.1 Example*

From the data of *Table 3-1*, streams can be organized into the following "thermo-physical compatibility" groups:

1. **{H1, H2, H5, C1}** for liquid, low viscosity, high density fluids;
2. **{H3, C4}** for liquid, high viscosity, middle density fluids;
3. **{H4, C3}** for gas of similar properties.

Note that:

- stream **C2** is likely not compatible with the first group of streams because of its high pressure, high temperature features. Therefore C2 shall not be a canditate for repiping a HEX designed for the first group of streams ... although a HEX designed for C2 could potentially be re-used for streams with less constraining features, while the reverse would clearly not be possible. This property demonstrates that the proposed approach based on the concept of groups of similar thermo-physical properties is actually a rather simplified method to specify the real opportunities to re-use HEX units.
- stream **C5** generally requires a specially designed HEX, not to be re-used by other streams.

### 3.2.3 Chemical Compatibility and Cleaning

The preliminary check for "thermo-physical compatibility" allows to significantly restrict the number of cases for which the chemical compatibility has to be verified, since only streams belonging to the very same "thermo-physical compatibility" group are concerned.

The concept behind the "chemical compatibility" is somewhat different from the "thermo-physical compatibility". There are actually three categories of "chemical compatibility":

1. total compatibility, between streams involving the very same fluid, or that feature unimportant differences (e.g. hot process water streams; milk and skimmed milk - both before or after pasteurization, to avoid biological cross contamination - , etc.). Total chemical compatibility means that cleaning is not required when switching between streams;
2. conditional compatibility, when a cleaning cycle is required either at the switching from, e.g., stream 1 to stream 2, or during the reverse change (2 => 1), or in both cases. Any cleaning is associated with costs: capital (cleaning system including control, valving and piping. etc.) as well as operational costs (energy, cleaning agents, event. labor costs);
3. incompatibility of streams, because either the cleaning would be too costly (or impossible), or various types of hazards could occur.

The common denominator of these three categories is the cost for changing from one stream to another one of the same "thermo-physical compatibility" group. Since actually the cleaning costs can hardly be calculated (or experience values are not available yet), the designer may distinguish between the following cases: • no cost; • low cost; • middle cost; • high cost; • very high cost.

The "no cost" option would be associated with "total compatibility", while "low cost", "middle cost", and "high cost" is meant to introduce ranking within "conditionnal compatibility". The "very high cost" option would pratically exclude the HEX re-use and mean "incompatibility".

Unlike the "thermo-physical compatibility", which is a transitive property and leads to the definition of groups, the "chemical compatibility" allows to define costs associated to transitions (switching) between the members (streams) within a group. These costs can conveniently be organized into a matrix format, as illustrated below.

Various heuristics could be developed to simplify the number of transitions to consider, since some of these might never take place. A severe restriction to the feasibility of some transitions originates from the batch schedule, as described in *Sub-section 3.2.4*. Although these schedule constraints are described separately to make a clear distinction between various types of "compatibility", in practice however, these constraints should be accounted for during the evaluation of the "chemical compatibility" so as to avoid assessing cleaning costs of impossible transitions.

In the general case, a HEX side can be used for more than two streams during a batch cycle. The costs associated with each "switch" between streams over a batch cycle should therefore be added. Note also that the re-use of HEX units between various streams may be associated with possibly significant piping/valving costs, which should be accounted for.

### 3.2.3.1 Example

The chemical compatibility is established for the streams within each group of similar thermo-physical properties:

1. within the first group **{H1, H2, H5, C1}**, H5 is supposed to include toxic release components which makes cleaning for HEX re-use with H1, H2 or C1 too expensive, or too risky. Cleaning costs for any transition between streams within the group are summarized in the following matrix format (*Figure 3-2*), where matrix elements shaded in grey represent

infeasible transitions (or transitions which are not meaningful, as elements on the diagonal):

**Group 1**

| Cleaning Costs | | to stream ... H1 | H2 | H5 | C1 |
|---|---|---|---|---|---|
| from stream ... | H1 | 0 | 0 | $CC_{H1H5}$ | $CC_{H1C1}$ |
| | H2 | 0 | 0 | $CC_{H2H5}$ | $CC_{H2C1}$ |
| | H5 | | | 0 | |
| | C1 | $CC_{C1H1}$ | $CC_{C1H2}$ | $CC_{C1H5}$ | 0 |

**Group 2**

| Cleaning Costs | | to stream ... H3 | C4 |
|---|---|---|---|
| from | H3 | 0 | $CC_{H3C4}$ |
| | C4 | $CC_{C4H3}$ | 0 |

**Group 3**

| Cleaning Costs | | to stream ... H4 | C3 |
|---|---|---|---|
| from | H4 | 0 | |
| | C3 | $CC_{C3H4}$ | 0 |

**Figure 3-2** Chemical compatibility, expressed as cleaning costs for transitions between streams (example process EP2).

2. similarly, cleaning costs for the second group **{H3, C4}** are expressed by a simple 2x2 matrix of which only two elements have actually to be evaluated;
3. within the third group **{H4, C3}**, H4 potentially includes toxic components, which prevent a cost-effective cleaning without risks, hence the element is shaded in grey.

As can be seen, the preliminary identification of groups of streams with similar thermo-physical properties allows to split the overall 10x10 matrix into smaller sub-matrices, reducing the number of stream transitions to consider.

Note that if a transition is not feasible, the transition in the opposite direction has to be excluded from consideration too, for consistency reasons (e.g. in group 1, transitions from any stream to H5, and in group 3, transition from C3 to H4).

### 3.2.4 Time Schedule Constraints for Repipe

The original problem of designing flexible HENs for continuous processes using the MBC approach (Jones, 1991), did not require the consideration of time schedule constraints. The base cases (operating modes) are supposed to be separated in time, or at least the HENs are operated over a long period compared to the "switching time" from one configuration to the next.

The cycle times of batch production processes are often in the range of hours, and the production volumes of high quality products are rather small. Changing the HEN configuration by repiping during operation of the related streams means disruption of the normal course, loss of valuable product (unless a complex pumping/draining system is provided), and generally requires a cleaning cycle (except in the case of total compatibility of the related streams, or when switching between heat recovery (soft data) streams). In conclusion, a safe strategy requires that repiping one HEX side be only possible at a time when no stream is flowing through this side, and provided that enough time (with a great probability) is available for the required cleaning cycle.

*Figure 3-3* illustrates a case of repiping one HEX side, and represents the

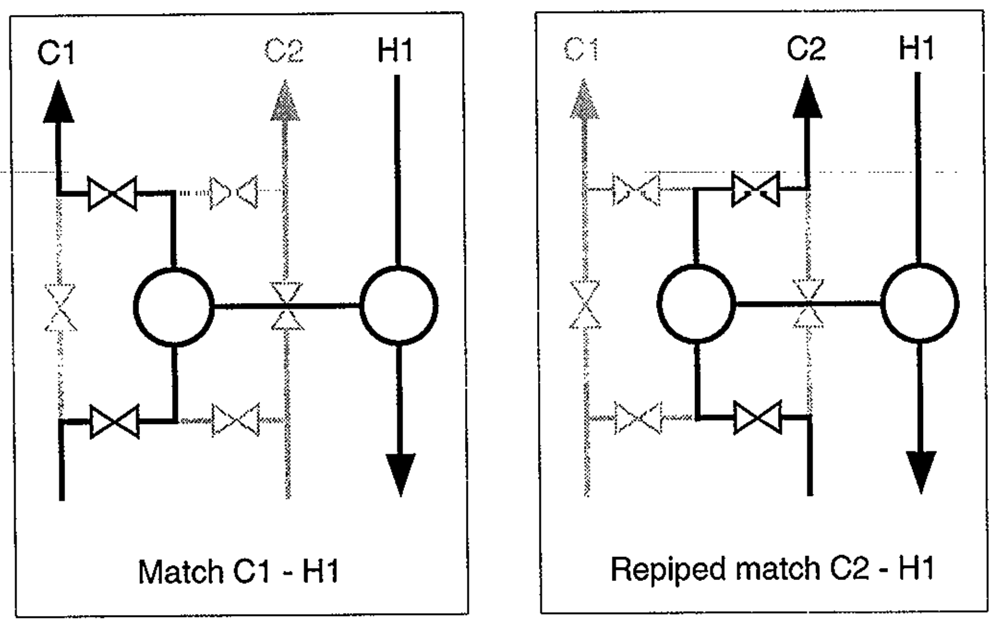


**Figure 3-3** Repiping a HEX on one side.

required piping and valving. At least six 2-way valves are needed for operation, while cleaning could require additional piping and valving.

### 3.2.4.1 Example

The feasible transitions represented on *Figure 3-2* are further restricted by schedule constraints (refer to the Gantt diagram of *Figure 3-1*):

1. **group 1**: focusing on the schedule of streams H1, H2 and C1, it appears that repiping from C1 to H1 (or the opposite) is not feasible, since C1 and H1 overlap in time. However, H1 and H2 do not overlap in time (with "sufficient margin"), as do C1 and H2, making the repipe feasible;
2. **group 2**: repiping from H3 to C4 (as well as the opposite) is feasible since these streams do not overlap in time;
3. **group 3**: repiping from H4 to C3 is chemically not feasible. Moreover, from the point of view of schedule constraints, this repiping would be difficult, since no time margin would be available for the cleaning process (although H4 and C3 do not overlap in time).

*Figure 3-4* represents the feasible repipe opportunities, taking into account both the cleaning constraints and the schedule constraints. Elements shaded in light grey are infeasible transitions from the schedule point of view. Depending on the use of this matrix of feasible transitions, various additional costs (piping, valving, etc) may be included.

| Cleaning Costs | | to stream ... H1 | H2 | H5 | C1 |
|---|---|---|---|---|---|
| from stream ... | H1 | 0 | 0 | $CC_{H1H5}$ | $CC_{H1C1}$ |
| | H2 | 0 | 0 | $CC_{H2H5}$ | $CC_{H2C1}$ |
| | H5 | | | 0 | |
| | C1 | $CC_{C1H1}$ | $CC_{C1H2}$ | $CC_{C1H5}$ | 0 |

Group 1

| Cleaning Costs | | to stream ... H3 | C4 |
|---|---|---|---|
| from | H3 | 0 | $CC_{H3C4}$ |
| | C4 | $CC_{C4H3}$ | 0 |

Group 2

| Cleaning Costs | | to stream ... H4 | C3 |
|---|---|---|---|
| from | H4 | 0 | |
| | C3 | $CC_{C3H4}$ | 0 |

Group 3

**Figure 3-4** Feasible repipe opportunities, taking into account cleaning and schedule constraints (example process EP2).

### 3.2.5 Time Schedule Constraints for Resequence

Resequencing does not require a cleaning cycle, nor does it imply losses of product, but changing the order of HEX units on a stream leads to transient conditions (on this stream and all streams which are matched "dowstream") which might not be tolerated, depending on whether the temperature control of the related streams is critical (e.g. for reaction) or not (e.g. pre-heating of non-biological stream, or intermediate stream for in-vessel heating or cooling).

Hence the feasibility of resequencing during operation is not only stream-dependant, but is a "downstream HEN" property which has to be assessed by the designer. Like for repipe, specifying resequence opportunities is a rather fuzzy activity left to the designer. However, the opportunity for resequence is time slice dependant, since the propagation of transient conditions depends of the "downstream HEN" active at the time of resequence.

Again, the specification of the resequence opportunities could be automated to a large extend, but this lays out of the scope of this project.

*Figure 3-5* illustrates a case of resequencing a pair of HEXs on a stream (H1) and represents the related piping and valving. At least three 3-way valves are needed; alternatively, six 2-way valves might be used.

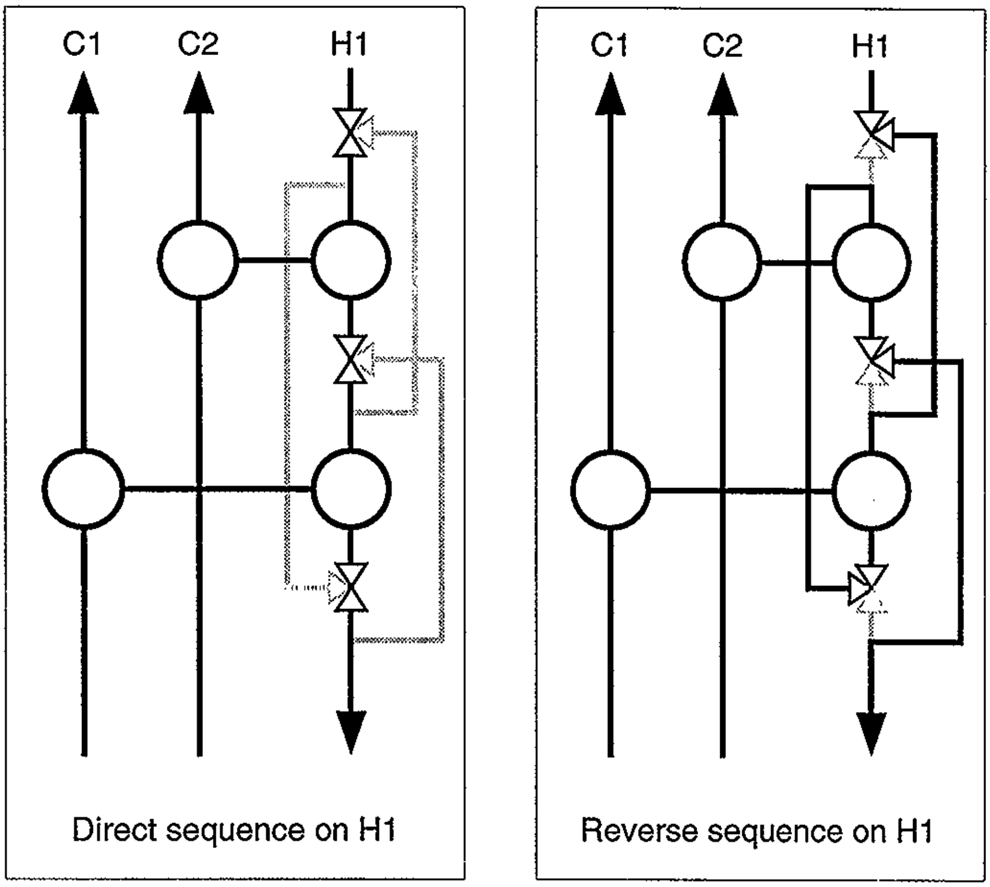


**Figure 3-5** Resequencing a pair of HEXs.

### *3.2.5.1 Example*

With respect to resequence, the following features are assumed for the example process:

- H4 and H5 are heat recovery opportunities and not process streams, hence they can be considered as insensitive to resequencing;
- C5 does not experience significant temperature changes (evaporation); therefore resequence is not needed on C5, while transient conditions resulting from resequencing on "upstream HEN" are tolerated;
- C2 and H1 are supposed to be "resequence insensitive" streams (i.e. their temperature control is not of critical importance, e.g. feed preheat or cooling);
- remaining streams (C1, C3, C4 and H2, H3) are supposed to be highly temperature sensitive and do not tolerate resequence (either directly on the stream, or within the "upstream HEN".

## 3.2.6
## By-pass to Reduce Active Heat Transfer Area

When re-used across several time slices, a HEX does not generally require (or make use of) the very same heat transfer area. Once designed to cope with the highest area requirement, partial by-pass of the HEX is needed to adapt to smaller area requirements.

As the adjustment of HEX area is an important aspect of the automated HEN design (refer to *Sub-section 3.3.6* on page 107), the following simple example, maybe quite obvious, is meant to illustrate the principle. It involves the case of the match M3 of example process EP1 (refer to Krummenacher & Favrat, 1995, p. 76). The size of M3 is set to 6.3 $m^2$ during the time slice 4 (refer to *Figure 3-6*, case a), while M3 is re-used between the same pair of streams for the time slices 1, 2 and 3 (*Figure 3-6*, case b), requiring only 3.9 $m^2$. With excess area on M3 (6.3 instead of 3.9 $m^2$), the target

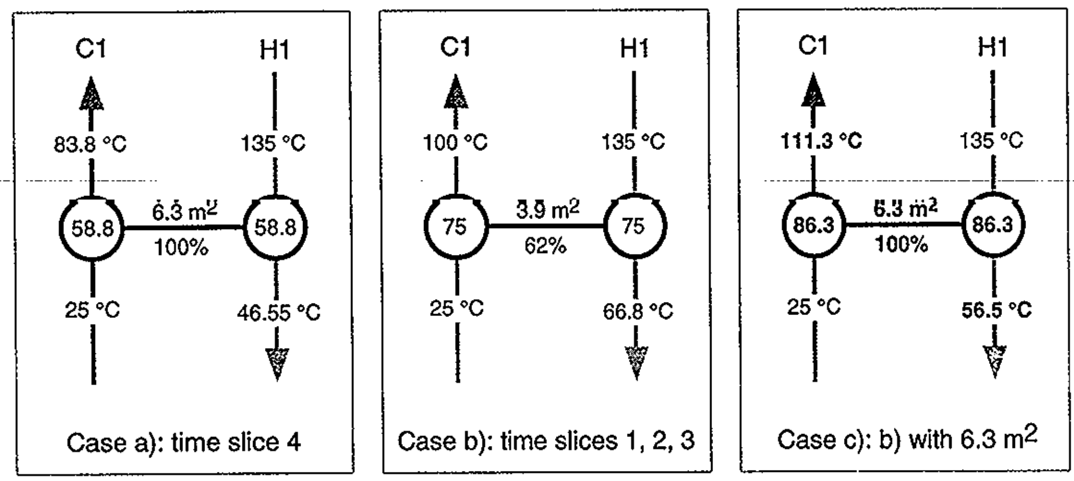


**Figure 3-6** Re-use of match M3 across time slices (see comments in the text).

temperature of stream C1 would be exceeded and C1 would then require cooling (*Figure 3-6*, case c).

*Figure 3-7* illustrates how the apparent area of M3 is reduced when by-passing part of the flowrate, and hence decreasing the effective $\Delta T_{lm}$. In this case, a by-pass factor of about 28% reduces the active area from 6.3 to 3.9 $m^2$. Note that the above case implicitly assumes that the heat transfer film coefficient is not influenced by the reduction of the flowrate through the HEX.

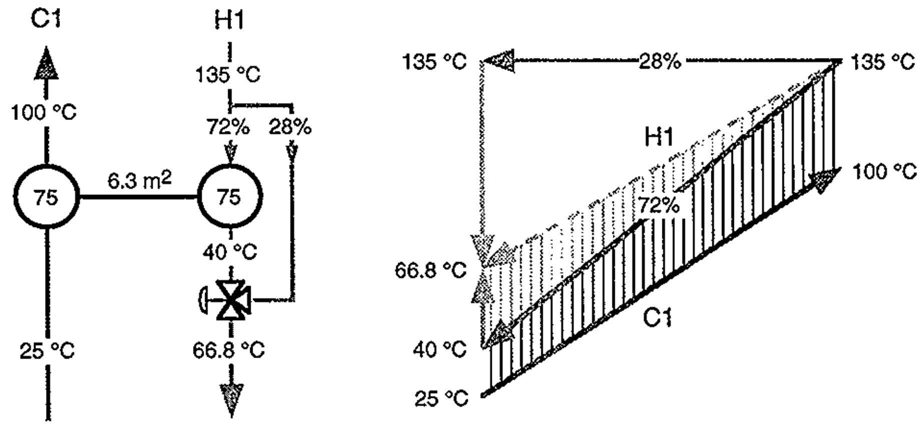


**Figure 3-7** Using a by-pass to decrease the active area of a HEX.

By-passing may be used on either side of a HEX. To select on which it is best applied in practice, the following criterias should help:

- temperature sensitivity: at the output of the by-passed HEX side, the "by-passed" stream is mixed with the "direct" stream (passing through the HEX). By definition, these two (sub-)streams are not at the same temperature: the "direct" stream "exceeds" the final mixing temperature, while the "by-passed" stream remains "below" the mixing temperature (refer e.g. to *Figure 3-7*). The extend to which the mixing temperature is exceeded can be a problem with temperature-sensitive products such as food products (brewing, dairy, etc.), bio-engineering products, flavour & fragrance, etc. The by-pass should preferably be used on the side where the corresponding stream is least temperature-sensitive;
- ease of cleaning: by-pass requires pipes and valves, which need to be cleaned. Some processes (in particular food processing) are subject to severe design guidelines which prohibit the use of control valves on steril product streams, since perfect cleaning of these valves is difficult to guarantee;
- sensitivity of film coefficient to a decrease of the flowrate: the by-pass should preferably be placed on the side showing the least sensitivity of the heat transfer film coefficient, in other words the side with the highest margin to laminar flow - particularly if this would be critical on the other side of the HEX;
- existing piping & valving: savings can be made on equipment costs if piping and valving for resequence or repipe already exist;

- required accuracy of temperature control: this criteria could also determine the side where by-pass should be applied.

Note that depending on the type of HEXs to be used and the required flexibility, a HEX unit could be split into several partial, serially connected, sub-units which areas match the various area requirements. In this way, and with on/off by-pass of unnecessary sub-units, the drawbacks associated with area adjustment using partial by-pass are avoided. On plate HEXs for example, this subdivision can easily be realized using intermediate ports (nozzles), while all plates are hold on one single frame.

# 3.3 Proposed Solution Approach Based on Genetic Algorithms

## 3.3.1 Introduction

The design & optimization of (continuous) heat exchanger networks actually involve two different (yet related) tasks:

- first the design of a HEN structure;
- then, given the structure, the search for the heat loads to optimize the objective function (e.g. the heat recovery, the total annual costs, etc.).

The first task is often referred to as being the structural optimization, which involves binary variables, while the second task is the parametric optimization, involving continuous variables (heat rate, heat transfer area, split fractions, etc.). Various ways to solve these tasks have been proposed so far (e.g. sequential or simultaneous, refer to *Section A.4* on page A-26, and *Section A.5* on page A-34). The distinction between these two different tasks makes sense in the context of batch HENs too, although these are to be found at two interrelated levels:

- at the level of each time slice, for which a feasible HEN structure and minimum utility costs (given maximum HEX areas) have to be identified;
- at the overall HEN level, i.e. the master HEN from which it should be possible to derive the feasible slice-wise HENs.

These two levels are interrelated since the various slice-wise structures have to be embedded in the master HEN, or, in other words, it should be possible to derive each slice-wise structure from the masterstructure using "structure transformations" which comply with the feasible repipe / resequence rules formerly discussed (refer to *Section 3.2* on page 80).

There are basically two possible approaches to address the structural optimization of batch HENs:

- a top-down approach, in which the overall HEN structure is first postulated, from which "consistent sets" of slice-wise structures are generated. In this context, a "consistent set" means that, within this set, any slice-wise structure is obtained from the preceding one through feasible repipe and/or resequence transformations (if any);
- or a bottom-up approach, which first addresses the design of slice-wise structures (independently), and then tries to generate a superstructure embedding each of the slice-wise structures.

The top-down approach has been foreseen as more appropriate than the bottom-up one:

- from a conceptual point of view, starting from the global HEN level and particularizing to slice-wise structures seems more reasonable and systematic than trying to identify a global HEN from the partial, not necessarily compatible networks;
- using the bottom-up approach, the number of HEX units of the resulting global HEN cannot be controled at the onset, since it is very much dependant on the structural similarities / dissimilarities of the independently generated slice-wise structures (e.g. if two slice-wise structures are similar and incorporate $U$ HEX units each, their "addition" towards obtaining the global HEN will at the best be made of $U$ units, while, if very dissimilar, the "addition" shall contain at worst $2 \times U$ units). According to Androulakis & Venkatasubramanian (1991) (refer to *Subsection A.5.2* on page A-34), the structural optimization using Genetic Algorithms (GAs) has been proved to be difficult in cases where the dimensionality of the space is constantly changing, i.e. when the number of HEX units is not fixed. In the top-down approach, the number of units can be fixed by the designer, providing him with a control of the HEN complexity.

Similar comments could be made with respect to the parametric optimization, confirming that the top-down approach seems to be more suitable.

Several methods for continuous HEN design & optimization based on GAs have been proposed (refer to *Section A.5* on page A-34). These procedures differ in their objectives, in the optimization scope assigned to GAs, in the way variables are encoded and in the GAs actually used. Most of the proposed methods use a GA based structural optimization, while the parametric optimization relies on deterministic methods based on mathematical programming.

For the problem at hand, a robust solution approach is searched for, i.e. the applicability of the approach should not depend on particular properties of the problem.

### 3.3.2 Working Principle of Genetic Algorithms

Genetic algorithms (GAs) have recently gained significant consideration in the engineering research community, as a robust method to optimize complex engineering problems, without requiring special mathematical features of the problem (unlike the deterministic solvers based on mathematical programming, which generally requires special features for the global optimum to be identified). Recent examples (not related to HEN design) can be found in Curti (1998), Olsommer (1998), and Pelster (1998).

A GA mimics, in a computational manner, the natural evolution of living species, where the fitest individuals (i.e. the one which are the most suited to their environment) have better chances to survive and reproduce, while other poorly adapted individuals tend to disappear on the long run. All characteristics of individuals are coded in the genetic material.

Unlike deterministic methods, GAs work with a population of individuals (solutions), which evolves over a number of generations through reproduction. Reproduction (i.e. propagation/evolution of characteristics) is mainly controlled by the strategy of fitness proportionate reproduction which promotes the survival of the fitest, i.e. the probability for an individual to be "copied" in the next generation is proportional to the degree to which he fulfills the objective function of the problem (=fitness factor). A small mutation rate allows to randomly explore the solution space for other potential solutions (to keep the diversity of solutions), while crossover combines existing characteristics of the "parents" (by random mixing) with the hope that the "children" will behave better than the "parents" by taking advantage of a combination of favorable features.

GA based optimization has the distinct advantage of providing the designer with a population of good solutions, not only with the single "best", from which he can choose according to additional criterias.

### 3.3.3 The Proposed Approach to the Design & Optimization Problem

The proposed approach to the structural & parametric optimization of batch HENs is schematically represented on *Figure 3-8*. It involves a decomposition of the optimization problem into two levels:

- at the upper level, the masterstructure as well as the HEX areas are designed and optimized using a GA;
- at the lower level, given the masterstructure and the HEX areas, the optimum consistent set of slice-wise structures and the corresponding minimum utility costs are searched for.

The approach includes the following main steps:

1. at the upper level, a population of master HENs (i.e. masterstructures and related HEX areas) is generated. Each individual is coded as a masterstring, including both integers (describing the structure) and reals (representing the area values);
2. from each masterstructure, and by making use of the "structural evolution" allowed by feasible repipe and/or resequence opportunities, an exhaustive set of slice-wise structures is generated for each time-slice. If neither resequence nor repipe are allowed, slice-wise structures are generated in a straightforward way since there will be only one slice-wise structure for each time slice. The more repipe and/or resequence opportunities, the larger the number of feasible slice-wise structures [1];
3. after exhaustive sets of slice-wise structures (for each time slice) have been generated, these remain to be organized into consistent sets (or sequences) of slice-wise structures. Let $n_{SWS,l}$ be the number of different slice-wise structures for time slice $l$ ($l = 1 \ldots L$).The number of consistent sets of slice-wise structures is actually not equal to the product $n_{SWS,1} \times n_{SWS,2} \times \ldots \times n_{SWS,L}$, but much smaller. This is so because once a slice-wise structure is chosen for time slice 1, the number of slice-wise

1. if a bottom-up approach was used, even in the simple case of one single slice-wise structure for each time slice (case of neither repipe nor resequence opportunities), it would be possible to generate several feasible masterstructures. In effect, merging of individual slice-wise structures can be made in various ways with respect to the sequence in which HEXs on a stream originating from various time slices are placed.

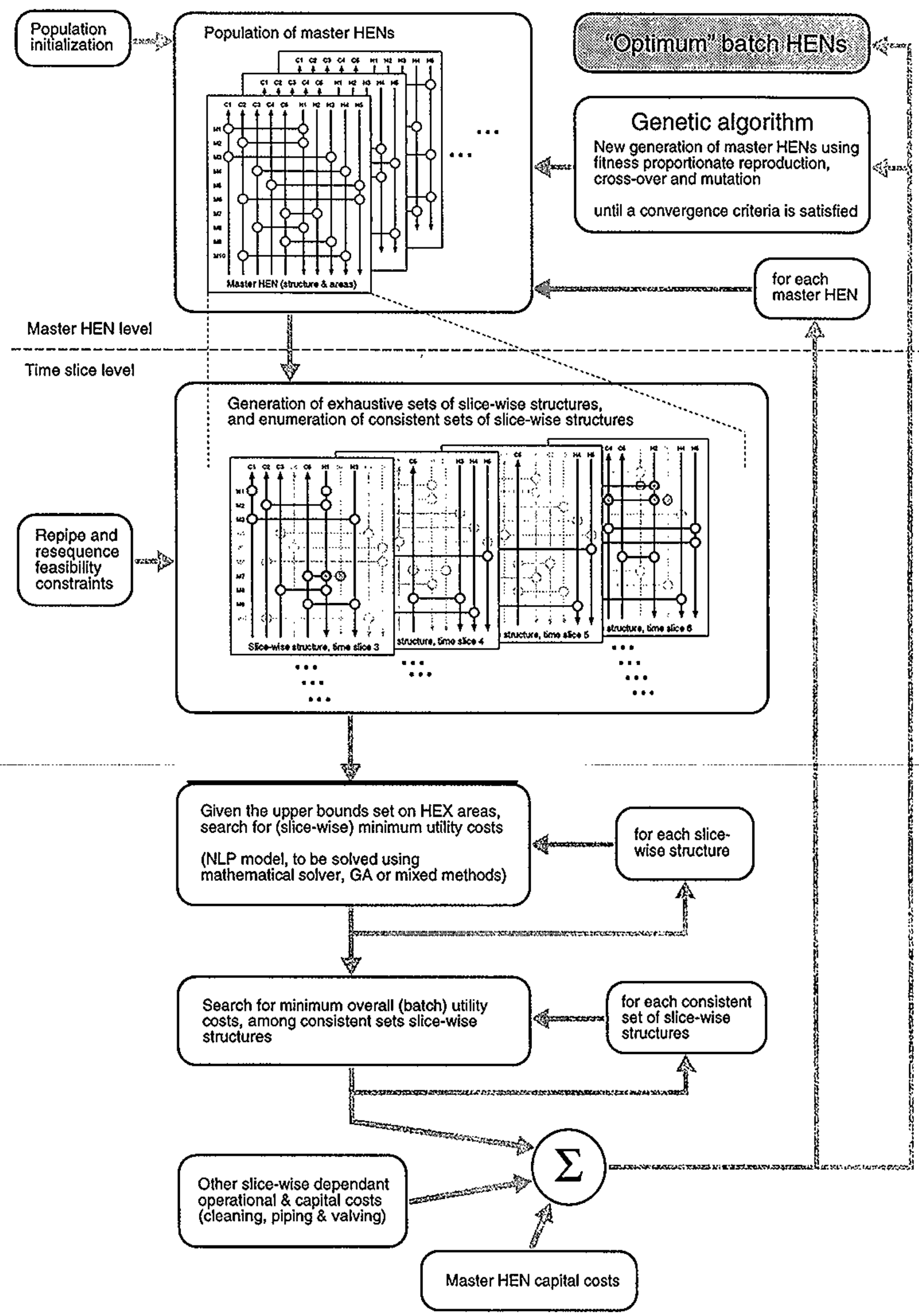


**Figure 3-8** Proposed approach to the design and optimization of batch HENs (see text for comments)

structures for time slice 2 which are structurally compatible (consistent) with the structure active during the former time slice is generally smaller than $n_{SWS,2}$, since structural changes by repipe can only take place in a time slice during which the related streams are not active (refer to *Sub-section 3.2.4* on page 85), or by resequence, when no streams sensitive to transient temperature conditions are present in the "downstream HEN" (refer to *Sub-section 3.2.5* on page 88). These compatibility conditions which restrict the structural evolution from one time slice to the next are not taken into account when generating the exhaustive sets of slice-wise structures. At the lower level, given the slice-wise structure and the maximum area for each HEX, the minimum utility costs are searched for each slice-wise structure. The problem is basically of NLP nature (refer to *Sub-section 3.3.6* on page 107 for more details); but depending on particular features of the model, a deterministic (MP) or stochastic (GA) optimization could still be considered;

**4.** once the minimum (slice-wise) utility costs are found for each slice-wise structure, the (overall, batch-wise) utility costs for each consistent set of slice-wise structures can be calculated; if related cleaning, piping and valving costs (which are slice-wise structure dependant costs) are added, the best performing ("fitest") set of consistent slice-wise structures can be identified (considering only the costs of the best set or averaging on several sets remains to be defined);

**5.** the minimum of slice-wise dependent costs is brought back at the upper level, where these costs are added to the capital costs of each master HEN individual, which allows to define the fitness factor of each individual;

**6.** the evolutionary strategy of the GA is applied on the population of master HENs, taking into account the formerly calculated fitness factor.

As already mentionned, the overall strategy has not been implemented yet. Several practical issues are therefore not fully defined, leading to the following comments:

- an algorithm able to efficiently generate an exhaustive list of consistent sets of slice-wise structures remains to be developed;
- unlike continuous HENs, for which heat rate would be prefered to define the matches, independent real (parametric) variables are the area value, since these are the actual values that remain unchanged, and since the maximum (design) values are not to be required during the same time slice. Specifying HEX areas instead of heat rate has the additional

advantage of leading to feasible HENs operation, whatever the actual (positive) area values (refer to *Sub-section 3.3.6* on page 107).

- as shown in the same *Sub-section 3.3.6*, finding the minimum utility costs for each time slice, given the maximum area of each HEX unit, is not a straighforward problem, since making use of the maximum area on all matches does not lead, in general, to the minimum energy costs. The active area of some matches have to be reduced using by-pass;
- the two-level approach is potentially well suited for parallel computing, in that searching for the minimum utility costs for a slice-wise structure is inherently independent of the calculation performed for other slice-wise structures. Parallelization is particularly desired at this level since this step is expected to be the bottleneck for the required computing time;
- as for any problem, there is not only one single, unambiguously identified solution method. In particular, it remains to be verified that the GA is inherently robust and "intelligent enough" to keep trace of good area values, and/or efficiently adapt to constantly changing masterstructures. If this would turn out not to be the case, a two-stage GA based optimization would be needed (at the upper stage, optimization of the masterstructure, while the optimization of HEXs area would be achieved at the second stage). At present, criterias do not exist for choosing between these two options;
- it also remains to be verified that when the number of units is chosen beyond a maximum number of HEX units (depending on the process), HEX units in excess of this maximum required number are automatically suppressed by setting their optimum area value to zero;
- the proposed GA optimization approach is based on given time slices, hence fixed scheduling. An outer loop should be included, so as to assess rescheduling opportunities (within given limits, for which suitable rules to specify the limits remain to be formulated). Sensitivity of solutions to schedule variations should also be analyzed.

#### 3.3.3.1 Example

*Figure 3-9* represents a possible masterstructure for example process EP2 (refer to *Sub-section 3.1.3* on page 77), including 10 HEX units.

Given this masterstructure, the Gantt diagram (refer to *Figure 3-1* on page 78) and the feasible repipe opportunities (refer to *Figure 3-4* on page 87)

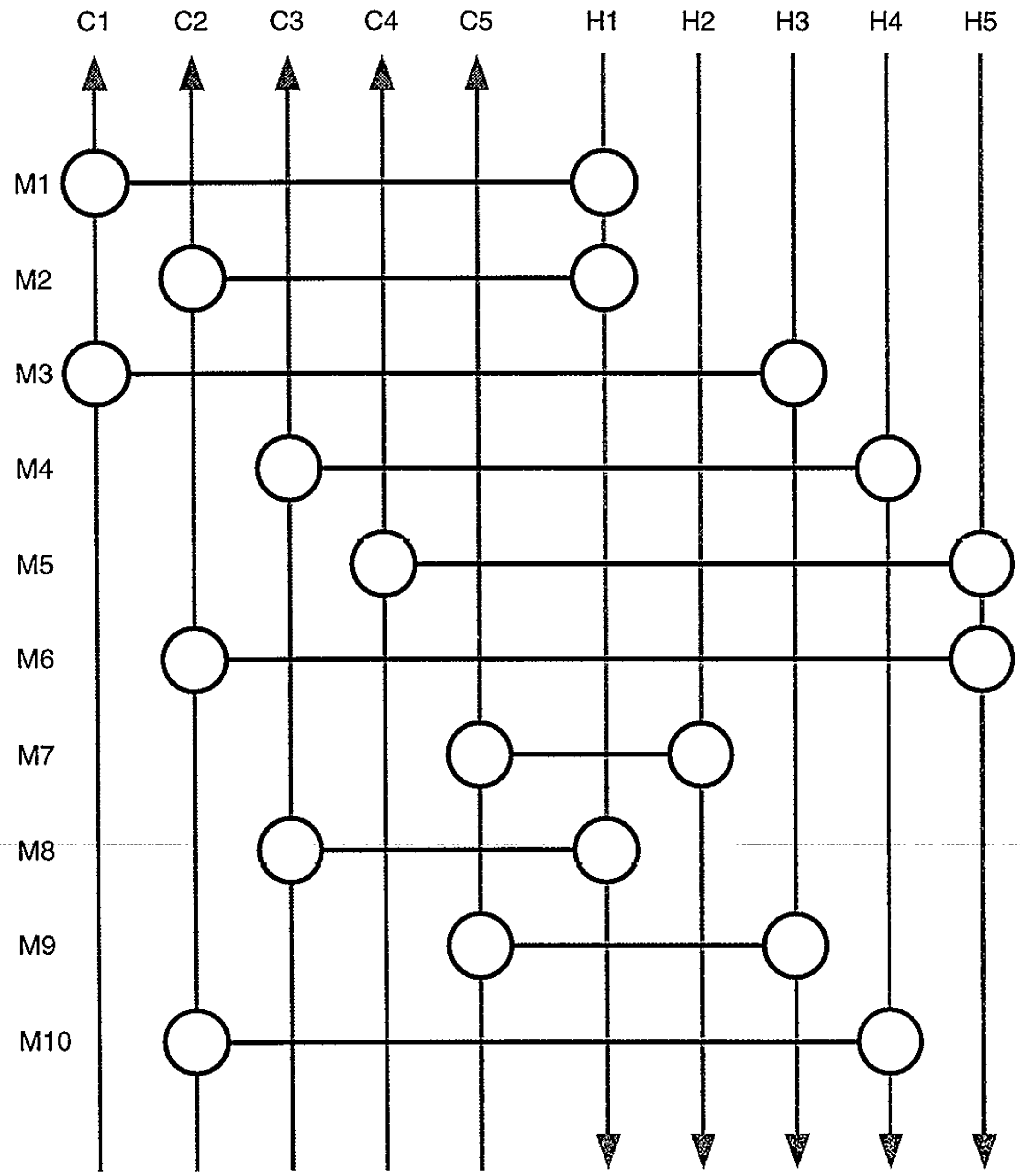


**Figure 3-9** A possible masterstructure for example process EP2.

allow to derive the following consistent set (or sequence) of slice-wise structures represented on *Figure 3-10* and *Figure 3-11*. With respect to repipe and resequence opportunities, the following comments should be made:

- time slice 1 (and 9): only one slice-wise structure is actually possible, no other HEX can be repiped, e.g. M4 (C3-H4) cannot be repiped from H4 to H1, as is the case for M1 (C1-H1) or M2 (C2-H1), which cannot be repiped on their cold side to C3;

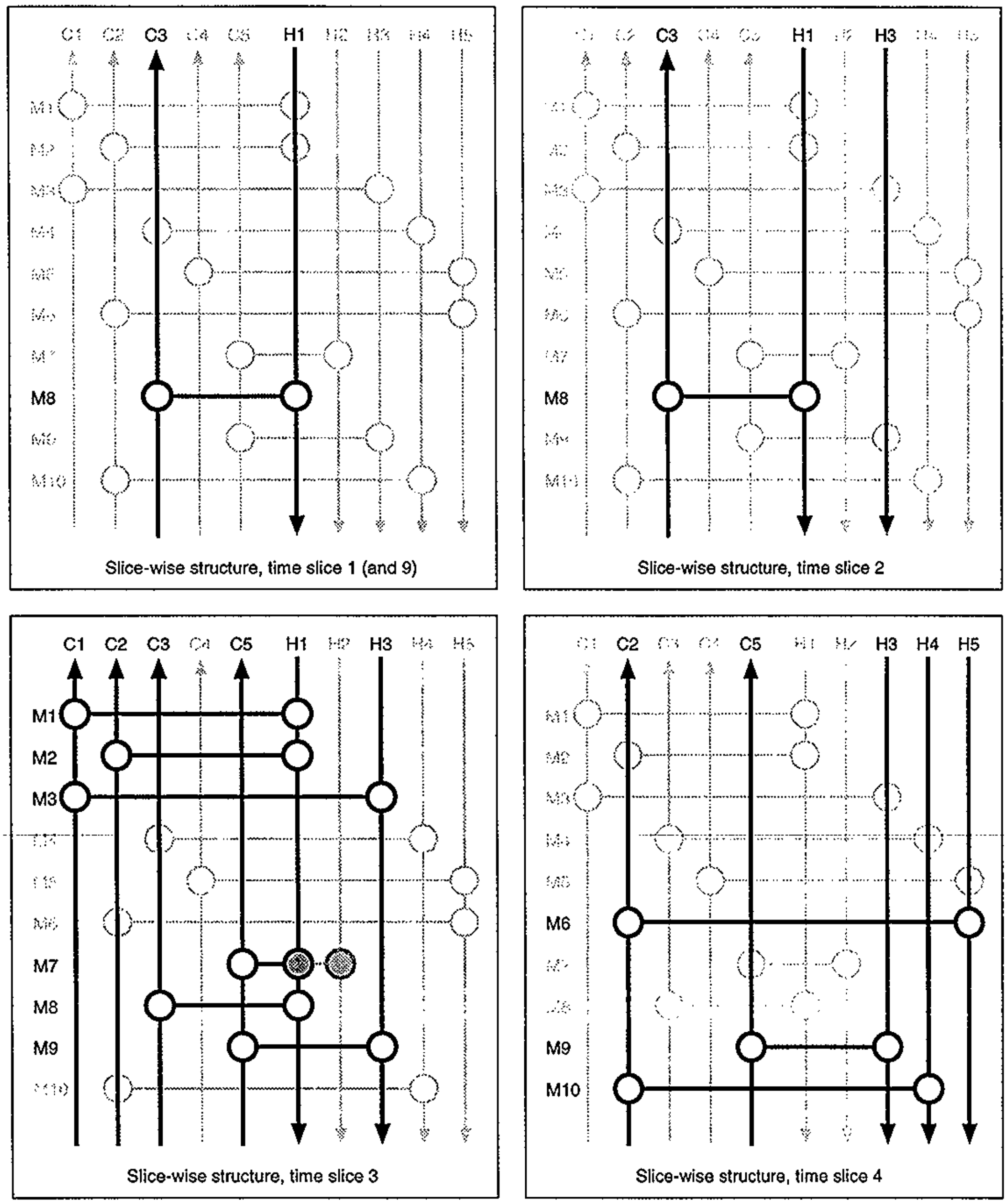


**Figure 3-10** Slice-wise structures (time slices 1 to 4, and 9).

- time slice 2: as for time slice 1, there is only one single possible slice-wise structure. The very same arguments hold, and additionally, neither M3 nor M9 can be repiped on their cold side to C3. Note also that resequence is not an issue, since there is only one HEX unit on the streams (not a sequence);
- time slice 3: the slice-wise structure shown on *Figure 3-10* includes the repipe of M7 from H2 to H1 (the "switching" from H2 to H1 has actually

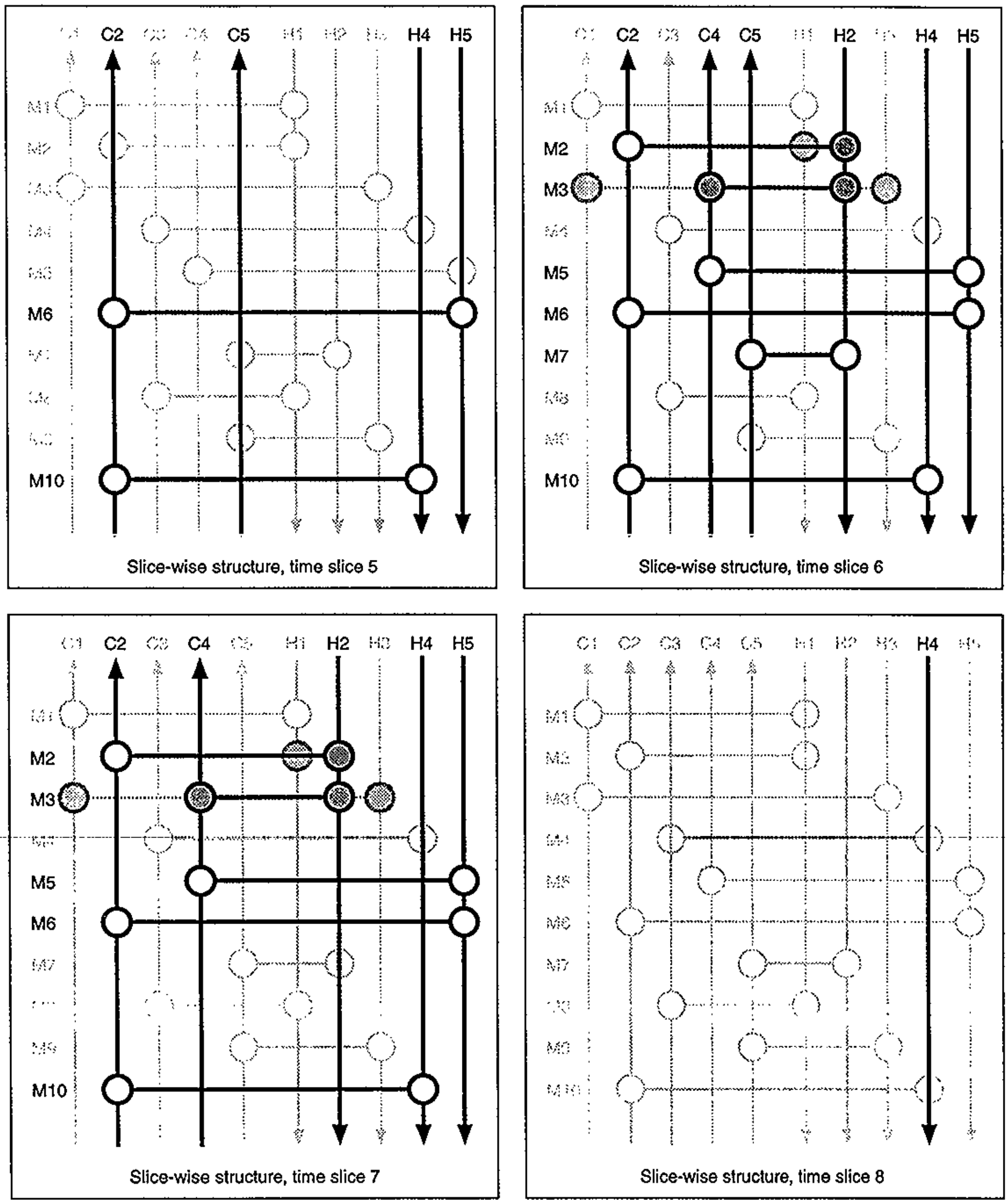


**Figure 3-11** Slice-wise structures (time slices 5 to 8).

been performed while H1 did not exist yet, i.e. during time slice 8 of the preceding batch cycle ). But one could have also decided not to repipe M7 at all, or repipe it in another place on the sequence of matches M1, M2, M8 (three additional possible positions). Hence, 5 possible slice-wise structures are associated with the repipe of M7. What about resequence opportunities ? On C5, there is no need for resequencing M7 with M9, since C5 is supposed to be an evaporàtion stream with low or almost zero temperature increase. Reasons pertaining to not resequencing M1 with M3 on C1, and M3 and M9 on H3, are more "tricky". On one hand, neither C1 nor H3 tolerate resequencing; on the ther hand, resequencing could be realized during periods when C1 is not active (e.g. time slices ≠ 3), or when H3 is not flowing. But since the HEXs M1, M3, M9, if resequenced, would be used only for time slice 3, these resequences would look like "permanent resequences", and are not to be considered as embedded in the present masterstructure. By "permanent resequence", it is meant that the related matches never operate (i.e. are never active) in their original sequence as provided by the masterstructure;

- time slice 4: resequencing M6 with M10 on C2 is feasible, since H4 and H5 are heat recovery opportunities (i.e. are not sensitive to transient temperature conditions), and since C2 is supposed not to be critical to transients conditions (e.g. pre-heating of a feed). Hence, there are 2 possible slice-wise structures. No other HEX can be repiped to be used during this time slice;
- time slice 5: considerations for time slice 4 still hold here; the fact that M9 is not active anymore is unimportant, because this match (C5-H3) is independant of C2, H4, and H5. Therefore there are also two possible slice-wise structures. It may also be interesting to note, for the consistency of slice-wise structures 4 and 5, that although it is theoritically possible to work with the sequence M6 -> M10 on C2 during TS 4, and with the reverse sequence (M10 -> M6) during time slice 5, this could not be justified in practice, because the temperatures conditions on the sub-system made of C2, H4 and H5 remain identical during both time slices;
- time slice 6: on *Figure 3-11*, both matches M2 and M3 are repiped. Repiping M2 (on its hot side from H1 to H2) could have occured during TS 4 or TS 5, when neither H1 nor H2 are present, and the reverse could occur during TS 8. Repiping M3 (on both sides, from C1 to H2, and from H3 to C4) require that no one of streams C1, C4, H2, H3 be active, which is the case during TS 5, and TS 8, TS 9, TS 1 for the reverse repipe. Since matches M2 and M3 are expected to be active during TS 3 in their original position (with respect to the masterstructure), these repipes are not, a priori, "permanent repipes". Note that M2 and M3 can be repiped in various sequences on H2. M3 may also be repiped in a reversed sequence on C4 (could also be placed upstream with respect to M5). Other resequence opportunities (not associated with repipe) could be found on C2 and H5. On C2, M6 and M10 could be found in a reverse sequence,

but resequencing could not take place during TS 6, since "resequence sensitive" streams are present in the matches (HEN) downstream on C2 (e.g. H2, C4). If required, the resequence could occur at the end of TS 5. On H5, the resequence of M5 with M6 would be a "permanent resequence": C4 (matched to H5 by M5) does not tolerate resequence, meaning that resequencing when C4 is present (TS 6 and TS 7) is not feasible (resequence could occur during any other time slice). But since a resequence of M5 and M6 would only concern TS 6 and TS 7, and the fact that a resequence during these two time slices is not feasible, a resequence of M5 and M6 (compared to the original sequence as from the masterstructure) would be a "permanent resequence", which is not acceptable (the reverse sequence of M5 and M6 will only be modeled by a related masterstructure). With the feasible repipe and resequence opportunities mentionned above (including the case when M2 and M3 are not repiped, i.e. are "inactive"), there are a total of 32 slice-wise structures for time slice 6;

- time slice 7: as for TS 6, M2 and M3 can be repiped, while M6 and M10 may appear in the original sequence or resequenced. Taking into account each feasible structural change leads to 16 slice-wise structures for this time slice.
- time slice 8: only H4 is present, so no process-to-process match can be used;
- time slice 9: as time slice 1.

The resequence and repipe opportunities have been intentionally discussed in details, so as to exemplify the issues. A systematic way of representing these opportunities, in the perspective of a computer implementation of the slice-wise structure generation, is obviously needed. This requires a modelization of resequence opportunities, in a way similar to the feasible repipe opportunities. But unlike repipe, resequence opportunities do not only depend on properties of the (directly) matched streams but also from those which are in the "downstream HEN".

Slice-wise structures obtained by "permanent" (or "systematic") repipe and resequence have been eliminated from the sets of slice-wise structures, in order to restrict the computational effort for the given masterstructure; the eliminated slice-wise structures are actually embedded in other masterstructures.

Summarizing the number of slice-wise structures for each time slice:

$n_{SWS,1} = 1$; $n_{SWS,2} = 1$; $n_{SWS,3} = 5$; $n_{SWS,4} = 2$; $n_{SWS,5} = 2$; $n_{SWS,6} = 32$; $n_{SWS,7} = 16$; $n_{SWS,8} = 1$; $n_{SWS,9} = 1$.

Without accounting for identical or degenerate slice-wise structures, a total of:

$$n_{SWS} = \sum_k n_{SWS,k} = 61$$

slice-wise structures have to be evaluated with respect to minimum (slice-wise) utility costs. If structural changes from one time slice to the next were not restricted (i.e. if the time slices were fully independent of each other), the (overall, batch-wise) utility costs would be the sum of the minimum obtained for each time slice - finding the minimum (among the different slice-wise structures) of slice-wise utility costs for a given time slice is straighforward task.

However, with respect to structural changes, the time slices are often not independent, due to the fact that repiping and/or resequencing can only occur during some specific time slices. As already mentionned, consistent sets of slice-wise structures have to be generated, and systematically evaluated in order to find the consistent set with the minimum overall, batch-wise, utility costs. To illustrate the concept of consistent slice-wise structures, consider the case of TS 6 and TS 7 (refer to *Figure 3-11* on page 101): repiping M2 and/or M3 from TS 6 to TS 7 is not feasible, hence consistent sets shall include slice-wise structures for TS 6 and TS 7 in which the matches M2 and M3 feature similar positions with respect to repipe (but not necessarily with respect to resequence, which obeys other kinds of restriction). Again, systematic methods to formalize the consistency rules need to be developed.

Note that the slice-wise structures for TS 3, TS 6 and TS 7 include more streams and HEX units that will most likely be found in real batch processes. Therefore the number of possible slice-wise structures for these time slices and the related combinatorial difficulties may in this case be overestimated.

### 3.3.4 Simplifying Assumptions

Compared to the Pinch Design Method, the HEN design approaches based on mathematical programming (refer to *Appendix A* on page A-26) features a significantly wider range of HEN structures, depending on the underlying assumptions. With most general superstructures or hyperstructures, complex HEN structures are obtained that feature numerous stream splits, by-pass, parallel / serial structures, and of course non-isothermal mixing. While the simplified superstructure approach proposed by Yee & Grossmann (1990), which assumes a stage-wise decomposition and isothermal mixing, leads to more simple, practical HEN structures, but potentially exclude some "tricky structures" that would appear more efficient, but more difficult to control. It is also interesting to note that whatever structural "components" in the HEN structure (mix and splits, non-isothermal mixing, etc.) are allowed or not, the optimum HENs obtained feature quite similar economical performances - although the structures might be very different.

Actually, simplifying assumptions are not only required to make the problem "easier" to solve, but also to control the HEN complexity. With respect to flexible batch HENs, complex optimal structures as those mentionned above are not desired - resequence and repipe bring already enough complexity !

It is assumed here that the stream splitting of process streams is not allowed, (at least to first demonstrate the feasibility of the approach). Parallel structures are therefore excluded, but these can generally be replaced by serial structure, at the expense of potentially requiring more HEN units.

In addition, the minimum temperature driving force (EMAT of $\Delta T_{min}$) is assumed to be very small (in the order of 0.5-1.0 °C), so as to avoid limiting the search space. This shall be used in the temperature driving force conditions when solving for the HEN operating conditions.

### 3.3.5 Coding the Master HEN

HEN masterstructures satisfying the above no-split assumption are easily encoded in the following way, proposed by Androulakis & Venkatasubramanian (1991) (refer to *Sub-section A.5.2* on page A-34):

given $I$ hot process streams and $J$ cold process streams, the structure of the HEN is described as a string of "characters", each "character" being one among the set (alphabet) of possible matches containing $I \times J$ characters .

For example, the masterstructure represented on *Figure 3-9* on page 99 is coded as the following masterstring, assuming the string begins at the hot side of the HEN and the match "character" is coded as $i - j$, i.e. hot stream numbering - cold stream numbering:

**{1-1, 1-2, 3-1, 4-3, 5-4, 5-2, 2-5, 1-3, 3-5, 4-2}**

With this coding convention, crossover (exchange of parts of the masterstrings) and mutation (change of one character in the masterstring) operators have a direct physical meaning.

An alternate coding technique would be the one of Lewin *et al.* (1998) (refer to *Sub-section A.5.3* on page A-36), based on the concept of HEN level. However, this technique has the drawback of being sensitive to the choice of key streams, and to the ordering of these streams, which prevent some structures to be feasible within a predefined number of levels. In other words, the number of levels is not a suitable parameter to represent the complexity of the network, or to control it.

The number of HEXs units is actually the direct control parameter of the HEN complexity. The designer often faces the problem of searching for optimal solutions of HENs featuring a specified number of units, which would not be possible with the concept of HEN level.

Note that the HEN masterstructure represented on *Figure 3-9* on page 99 can be coded by several masterstrings, since, e.g., the HEX M3 (3-1) is free to be moved "between" HEXs M1 (1-1) and M9 (3-5), without actually changing the masterstructure, although it looks different, as does the corresponding masterstring. This is mainly a representation problem of the HEN; but it also means that some masterstructures have more chance (compared to other masterstructures) to be generated since they are coded by more strings representing the very same structure.

Although the above multiple coding problem should not be a major issue in the GA optimization, it might be helpful to define additional rules for the coding, closely related to the ability of identifying equivalent masterstrings.

One possible ordering convention would be to organize the masterstring so as to list the HEXs with lowest possible hot stream number first, which leads to:

**{1-1, 1-2, 2-5, 3-1, 3-5, 4-3, 1-3, 4-2, 5-4, 5-2}**

which looks quite different from the former masterstring.

### 3.3.6
### Calculating the Maximum Energy Recovery for Each Time Slice

Given a consistent set of slice-wise HEN structures (embedded in the masterstructure) and HEX area values, the aim of this step is to assess the fitness of the solution by identifying the energy cost savings actually possible with the set of HEX area values, i.e. how cost-effective these area values are.

The problem of finding the minimum utility costs given a structure and a set of area values can be described (for ease of understanding) as a twofold problem:

- first identify the state of the network when using the given area values;
- reduce part (or all) of the area values to reach the minimum utility costs.

Unlike the case when heat rates are specified (which may lead to temperature infeasibilities because of driving forces < 0 °C), specifying area values never leads to infeasible heat exchanges. Given the supply temperature of the streams and the exchange areas, the HEN temperatures will evolve to a stable operating point, where the target temperature of some streams might be "exceeded", meaning that cold streams have to be cooled and/or hot streams have been cooled to a point that they require heating. Some HEX units may also exchange heat in the reverse direction (i.e. from cold stream to hot stream).

In order to avoid excess cooling of hot streams, and/or excess heating of cold streams, the area of some HEXs have to be reduced. But in the general case, identifying which areas should be reduced (and how much) is not straightforward (while the case of independent HEXs is readily solved). The following example demonstrates that even for the simple case of 3 process HEX units, finding the optimal area values is not an obvious task.

At this point, systematic methods to address this problem have not been identified yet. The very first examples indicate that some guidelines could be established based on the structure of the network, but more analysis work is required. One could also make use of sensitivity tables and downstream paths (Kotjabasakis, 1988).

With respect to the search for actual area values which minimize the energy costs, the following aspects should be taken into account:

- the target temperature of process streams is specified, while this is not the case for heat recovery streams;
- although sometimes beneficial to reduce the area of utility HEXs, the use of reverse utilities should be prohibited in any case (pinched process as well as threshold process), which corresponds to imposing the following constraints: $CU \geq 0$ for hot streams, $HU \geq 0$ for cold streams.

Given a HEN structure, finding the maximum energy recovery (or least utility costs) for a given set of upper boundary values for areas consists of a NLP problem, in which the non-linearity exclusively arises from the constraints on the upper boundary values for areas. In this NLP model, the independent variables are the heat rates of process HEXs.

A priori, the NLP problem may be addressed either with a deterministic solver, by a GA approach, or by an hybrid methods, e.g. the "Extended Genetic Search" (Androulakis & Venkatasubramanian, 1991).

#### 3.3.6.1 Example

Consider the following stream table representing one time slice of a process (*Table 3-2*). A possible HEN structure, including 3 matches, is shown on

| Stream Name | T in [°C] | T out [°C] | MCp [kW/°C] | Heat Rate [kW] | h [W/m2°C] |
|---|---|---|---|---|---|
| C1 | 25 | 170 | 10 | 1450 | 2000 |
| C2 | 90 | 210 | 15 | 1800 | 2000 |
| H1 | 160 | 40 | 20 | -2400 | 2000 |
| H2 | 250 | 120 | 12 | -1560 | 2000 |

**Table 3-2** A time slice including 4 process streams.

*Figure 3-12* in four cases:

**a)** case before area adjustment, i.e. when total available area for each match is used, leading to the fact that the target temperature of C2 is exceeded, requiring cooling;

**b)** case where the target temperature of C2 is satisfied by adjusting the area of M3;

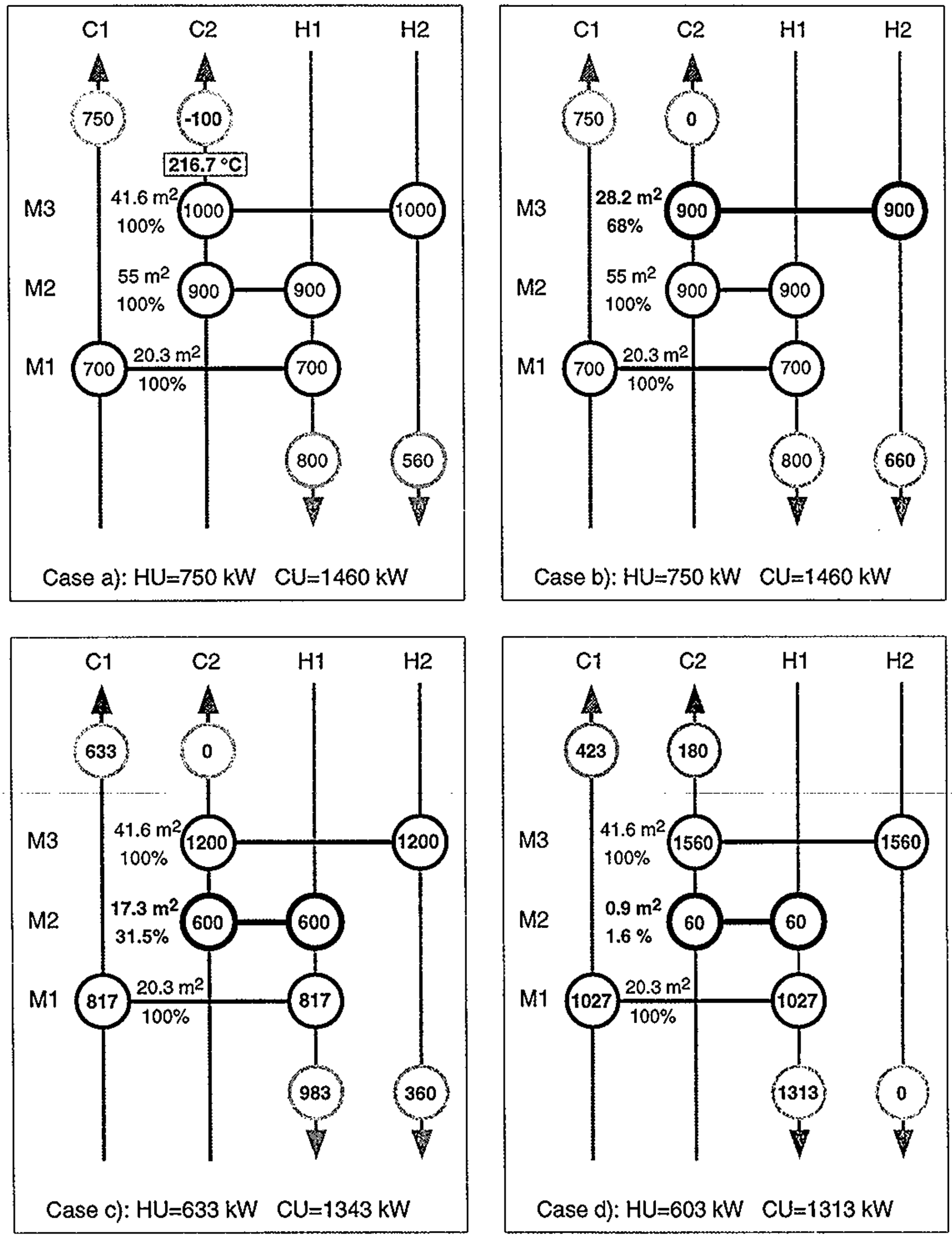


**Figure 3-12** Base case HEN (a) and three possible area adjustments (b, c, d) (see comments in the text)

**c)** case where the target temperature of C2 is satisfied by adjusting the area of M2

**d)** optimal case of area adjustment using the Excel Solver, showing that the objective function (the costs of utilities subject to the constraints of no reverse utility) can be improved by further reducing M2 area, up to a point where hot utility on C2 is needed, while the cooling requirement of H2 cancels out.

## 3.4 Simplifications for Both the Targeting and the HEN Design Stages

### 3.4.1 Motivation

This chapter has focused on automated strategies for direct batch HEN design and optimization. The proposed method complements the formerly developed MBC supertargeting algorithms, but does not replace them. Supertargeting is still a valuable tool at the conceptual design stage.

The number of time slices is an important issue for both the MBC supertargeting and the automated HEN design stages. The time slices divide a batch process in as many cases to analyse; any engineer will find this decomposition (although basically correct) particularly confusing, not allowing him/her to get an overview. The larger the number of time slices, the more complicated the analysis (e.g. a simplified model of a brewery process features not less than 18 time slices, while a realistic model would require about 25 slices, with several slices smaller than a few minutes !). There exists therefore a strong incentive to bring back this large number of slices to a more limited number of "fundamental" time slices, neglecting small or unsecure time slices (i.e. slices sensitive to schedule variations) which cannot justify an additional process-to-process (HR) HEX and/or a rearrangement of an HEN on the basis of expected energy savings. Any change in a HEN produces transient conditions, and possibly loss of product (the duration of the transient conditions depends e.g. on the inertia and product capacity of the HEX, the pipe length, etc.). The duration of the transient conditions should be reasonably small compared to the duration of the time slice, since transients generally mean the use of the related equipment in off-design conditions, i.e. non-optimal conditions.

### 3.4.2 Guidelines for Reducing the Number of Time Slices

A few guidelines have been identified so as to minimize the number of time slices, organized in the following reasonable strategy:

- first eliminate "artificial", meaningless time slices generated by streams not relevant to the process-to-process heat integration, or by soft streams;
- second, identify highly schedule sensitive times slices and suppress them;
- third, neglect streams of small duration and/or small heat content;
- finally, consider simple rescheduling opportunities allowed by existing equipment (synchronization of streams using available storage capacities of process vessels).

The guidelines of the first category are:

1. the obvious preliminary condition is to define the period of analysis (batch cycle) so that either its start or stop time coincides with the start of stop time of a process stream. In this way, the number of time slices is decreased by one unit (e.g. consider *Figure 3-1* on page 78, where time slices 1 and 9 are actually strictly identical !);
2. any process stream which is not included in the heat recovery region of TAM composites (time slice composites could be used instead, in particular if indirect heat recovery shall not be used, or feasible rescheduling of the stream has already been considered), at $\Delta T_{min}=0$, can be removed from the Gantt diagram, so that the start and stop times of this streams are no more deciding for the time slice decomposition;
3. soft streams (e.g. heat recovery streams, or storable process streams) should not be considered as deciding for the time slice decomposition. As a rule, heat recovery opportunities should first be excluded from the process TAM composites (time slice composites could be used instead, in particular if indirect heat recovery shall not be used, or feasible rescheduling of the stream has already been considered), so as to identify the location of the process pinch (or time slice process pinches, respectively). Only the part of HR opportunities above the process pinch should be included (the reverse rule holds for sub-ambient processes). Since the pinch location depends on the selected $\Delta T_{min}$, the lowest pinch location for a the reasonable minimum $\Delta T_{min}$ value should be considered (note that if only direct heat exchanges are considered, the global TAM pinch is not representative of the slice related $\Delta T_{min}$). Since a heat recovery stream is not a compulsory process stream, the related start or stop time are soft as well (the heat recovery can start later than the start of the stream, while the HR can stop earlier than the actual stop of the stream). On a Gantt diagram, heat recovery streams and related time lines

should be represented in a different stroke or color, to recall this property. In the case of storable process streams, such as hot process water, their start and stop times (corresponding to the period of actual use) have little to do with the time period they are actually prepared (in the proposed batch stream data table - refer to *Table B-1* on page B-8 - this property is formalized as possible *rescheduling* , with additional data for *delay*, *advance* and *modify rate* fields). Since their start and stop times are soft, they are best defined so as to match existing streams with fixed schedules. By doing so, storable process streams are not deciding the time slices anymore;

4. critical process streams for which the engineer knows at the onset that they need to be supplied by utilities (e.g. for controlability/quality reasons) are also eliminated from the heat integration problem, hence from the definition of the time slices (such streams are specified as *no integration* in *Table B-1* on page B-8);
5. in the absence of indirect heat recovery, any time slice featuring only streams of the same type (hot or cold) is not of interest to the heat integration analysis and can be ignored for the HEN design problem (it simply adds a constant to the total annual costs). This is the case of time slice 8 from the EP2 problem (refer to *Figure 3-1* on page 78).

The second category (schedule sensitive time slices) are mainly concerned with time slices which "short duration" (relatively to other time slices) is not due to corresponding short streams, but rather because a stream appears slightly before another one ceases to exist (or reversely). Assuming a significantly shrunk time scale of EP2 for the consistency of the discussion (refer to *Figure 3-1* on page 78), time slices 4 and 8 are examples of this kind of "small duration" time slices:

- time slice 4 is generated by the slightly delayed stop time of stream H3. From the point of view of H3, the stop time of H1, C1 and C3, and the start time of H4 and H5 are advanced. However, since H3 is the only stream which time deviates from the other ones, this stream is obviously responsible for the existence of time slice 4, and not the other streams responsible for the early end of time slice 3. In case of schedule variation, stream H3 could possibly stop earlier (downto the stop time of C1 and C3, making the slice 4 to disappear. One could, more likely, also argue that the scheduling of any stream among H1, H4, H5, C1 and C3 might change, which would introduce a new time slice. Regarding time slice 4, if the effective heat recovery opportunity offered by H3 during this slice is small (either because of a small duration or of a relatively small heat rate, or because of unfavorable temperature level for heat recovery), one would neglect the part of H3 during this slice by assuming it is satisfied by cold utility, i.e. time slice 4 would be neglected. The schedule variation of the other streams around the end of time slice 3 is most likely, since this is defined by a conjuction of unrelated (i.e. not synchronized by a "master/ slave" relation), and this should be solved by utility and utility HEX (if not already needed for other slices).

- time slice 8 is defined by streams H1, H2, H4, C2, C3 and C4. Stream H4 is the only stream present during this slice, hence it has to be matched with the cold utility, and the time slice eliminated from the heat integration analysis (according to guideline 5) described above).

Three potentially associated problems to such times slices can be mentionned:

- the high sensitivity to schedule variation which make the calculated heat recovery potential unlikely;
- relatively significant transient effects;
- a low potential heat recovery potential, or more generally low potential annual costs savings.

There is therefore an obvious need for criterias to decide whether a time slice has to be taken into account or can be neglected. Two different criterias can be formulated:

6. a time slice $\mathtt{1}$ which absolute duration is smaller than a threshold duration should be neglected:

$$\Delta t_{\mathtt{1}} \leq \Delta t_{min} \tag{3-1}$$

this constraint of minimum duration takes primarly the controllability/ transients effects into account; the threshold duration $\Delta t_{min}$ value depends on plant and process parameters. It should be possible to get likely values from process operators.

7. for a time slice which satisfies the condition of minimum absolute duration (i.e. $\Delta t_{\mathtt{1}} \leq \Delta t_{min}$), it remains to be verified that the heat recovery potential associated with the stream(s) which generates it is not too small relatively to other times slices. Various criterias can be formulated, e.g:

• the relative duration of the time slice, i.e. the ratio of its duration over the batch cycle, which criteria is very easily calculated. With respect to contribution to heat recovery, this criteria implicitely assumes that the rate of heat recovery is almost independant of the time slice, i.e. uniform over the batch cycle ... maybe too crude an assumption;
• or a detailled estimation of the benefit to cost ratio associated with the stream(s) responsible for the definition of this slice (accounts for the ability of this slice (more precisely the stream(s) which defines it) to significantly contribute to the objective function. Such a criteria may be more robust, but requires more computer time, and, if it is to be used before MBC supertargeting, is still plagued with fundamental limitations (such as the by-default constant $\Delta T_{min}$ assumption and the inability to account for the re-use of HEX units and the related capital savings).
A simple criteria is proposed, which is based on the criteria first mentionned (i.e. the relative duration of the time slice) yet corrected to account for the relative contribution to overall heat recovery. This allows for cases where there exists long periods with no heat recovery potential, while heat recovery is essentially concentrated in small time slices (a case which is not so seldom in batch processing). Let's define:

$$RB_{\mathtt{p},\mathtt{1}} = \left.\frac{\Delta t_{\mathtt{1}}}{\sum_{l}\Delta t_{l}} \cdot \frac{\Delta HR_{\mathtt{p},\mathtt{1}}}{\sum_{l} HR_{l}}\right|_{\Delta Tmin_{l} = cte} \quad (3\text{-}2)$$

where:

- $RB_{\mathtt{p},\mathtt{1}}$ is the relative benefit of considering the contribution of process stream $\mathtt{p}$, responsible for the definition of time slice $\mathtt{1}$, in the heat integration;
- $\Delta t_{\mathtt{1}}$ is the duration of time slice $\mathtt{1}$;
- $\sum_{l}\Delta t_{l}$ is the period of analysis, i.e. the batch cycle time;
- $\Delta HR_{\mathtt{p},\mathtt{1}}$ is the contribution of process stream $\mathtt{p}$, during time slice $\mathtt{1}$, to the heat recovery. $\Delta HR_{\mathtt{p},\mathtt{1}} = \Delta HR_{\mathtt{1}} - \Delta HR_{p \neq \mathtt{p},\mathtt{1}}$ where $\Delta HR_{\mathtt{1}}$ is the heat recovery contribution of time slice $\mathtt{1}$ with all process streams included, for a given $\Delta T_{min}$, while $\Delta HR_{p \neq \mathtt{p},\mathtt{1}}$ is the the heat recovery contribution of time slice $\mathtt{1}$ with all process streams except stream $\mathtt{p}$;
- $\sum_{l} HR_{l}$ is the overall heat recovery, with all process streams included, for the period of analysis. The heat recovery of each time slice is obtained with a single $\Delta T_{min}$ (e.g.

$\Delta T_{min}$=10 °C). A high sensitivity of $RB_{p,1}$ to the actual $\Delta T_{min}$ might indicate a poor confidence in the proposed criteria.

The criteria for "neglecting" time slice $\mathbf{1}$ defined by process stream $\mathbf{p}$ is expressed by:

$$\frac{RB_{p,1}}{\sum_{l} RB_l} \leq \varepsilon_{RB} \tag{3-3}$$

where:

- $RB_{p,1}$ is defined by *Equation* 3-2 above;
- $\sum_{l} RB_l$ is the overall relative benefit of all time slice; individual $RB_l$ are calculated using *Equation* 3-2, but with $\Delta HR_1$ instead of $\Delta HR_{p,1}$ (i.e. the relative benefit of all process streams in the time slice $\mathbf{1}$);
- $\varepsilon_{RB}$ is the relative benefit threshold value (e.g. set at some value in the range 0.02-0.1).

If not a single, but several streams are responsible for the definition of the time slice $\mathbf{1}$, the relative benefit defined by *Equation 3-2* is evaluated globally for these streams.

Streams of small duration (third category) can also be analyzed with the same *Equations 3-2 and 3-3.*

### 3.4.3 Comments

It is important to clarify what is meant by "neglecting" a time slice on the basis of *Equations 3-2 and 3-3*. Neglecting does not mean ignoring what actually happens during this time period, in particular the heat recovery allowed by the streams $p \neq \mathbf{p}$ that exist during this slice and do not stop define this slice (e.g. streams H4, H5, C2 and C5 during time slice 4 of the EP2 process - refer to *Figure 3-1* on page 78). It simply means that stream H3, which stop time defines time slice 4, should be supplied by the cold utility from time 300 to 340, and since H3 does no more define the time 340 as a time when the stream population (for heat recovery) changes, the original time slice 4 disappears and a new, longer time slice from time 300 to time 420 is now defined.

The relative benefit expressed by *Equation 3-2* accounts for the heat recovery (the contribution which decrease the total costs) and the time needed to recover this heat: the longer the best, since the area (and hence the capital costs) are minimized. It is implicitely assumed that the capital costs associated with heat recovery are uniform, which is generally not the case (because of different temperature driving forces, of HEX re-use, etc.). If the heat transfer film coefficient features large variations between process streams, it could be introduced as a correction factor in *Equations 3-2 and 3-3.*

Although guidelines can be specified, the preliminary simplification of the process schedule requires judgement and there isn't a single right way to make this simplification. Not only small time slices and the streams responsible for these have to be identified, but also potential new time slices due to schedule variations should be anticipated. Note also that in-vessel streams featuring large temperature variations may need to be time segmented and increase the number of time slices.

Depending on the remaining complexity/number of time slices left after a first simplification, a more severe threshold value $\varepsilon_{RB}$ might be required (the threshold value to reduce the process to a L time slices is not known at the onset.

A potentially more fundamental reason to bring back the process schedule to a limited number of "essential" time slices should be mentionned: if small time slices are kept in the specification of the automated HEN design and optimization problem using GA, this specification is constraining and potentially prevents resequence and/or repipe to take place for "essential" time slices. Eliminating these small time slices can help to find better re-use of HEX units. Then, the population of "optimal" solutions provided by the GA should be analysed with respect to their additional ability to integrate the previously excluded streams by re-using otherwise unused HEX units. Hopefully some solutions will allow this; in the opposite case, the user may decide to include the stream in the heat integration and launch another design/optimization run.

### 3.4.4 PinchLENI and Mixed Modes of MBC Targeting

Although it has not been possible using PinchLENI to address processes with a large number of time slices (due to numerical issues in the Simplex algorithm), preliminary analysis indicates that the supertargeting might be difficult or fail to identify good individual pinches and costs targets for small time slices, because of the modeling limitations stating either conventional or resequence, but not both. This could also be a consequence of the calculation model assuming vertical heat transfer between composites.

Improving the MBC supertargeting algorithms would be mainly concerned with the use mixed supertargeting (partly repipe, partly resequence). This is unfortunately essentially not possible, unless the process streams can be reasonably separated in two isolated sub-systems, for which we could select the best suitable mode of HEX re-use.

But the proposed compatibility matrix (thermo-physical & chemical & scheduling) allows to assess whether a signifiant number of cases allows repipe, or whether HEX re-use should be limited to resequence. Whatever the HEX re-use mode actually assumed, the MBC supertargeting assumes vertical heat transfer !

## 3.5 Conclusions

A GA-based approach to the design and optimization of direct batch HENs has been proposed. As a result, a population of near optimal batch HENs shall be provided, from which the user may choose according to additional criterias. The solution approach includes a decomposition into an upper level, where the structure of the overall HEN (the masterstructure), as well as the area values, are optimized, and a lower level which optimizes the use of the given HEX units for each time slice, in terms of both structure and actual HEX areas. Although several important issues have already been addressed, the methodology remains to be implemented and validated.

As far as HEX re-use modes are concerned, rules pertaining to batch processes have been formulated under the form of repipe and resequence compatibility matrices. These matrices, which mainly formalize practical constraints (thermo-physical properties, chemical/cleaning properties, and schedule related constraints), severely restrict the number of feasible repipes or resequences, respectively. This is a desirable prerequisite for the application of the GA based approach, since a high degree of feasible repipe would cause the combinatorial complexity of generating the slice-wise structures to burst out. In principle, the methodology is also applicable to multi-product and multipurpose batch plants, as well as to MBC design for flexible continuous processes, provided that the cleaning and schedule contraints limiting repipe or resequence are adapted accordingly.

Restricting the time slices to most "essential" ones is an important issue for both the supertargeting and the design stage. Guidelines, organized into a simple strategy, to identify meaningless streams and time slices have been developed.

As already highlighted, one of the main drawbacks of direct heat integration is the sensitivity to inevitable variations of schedule. This important aspect is not taken into account in the GA based optimization; a sensitivity analysis to schedule variations should be performed a posteriori for the various HEN solutions provided, and hopefully some suitable HEN might be identified. It could be possible to take these issues into account during the optimization process by specifying forbidden matches, provided that a methodology is developed to identify the critical matches with respect to schedule variations.

To make the automated synthesis approach using GA robust and generally suitable for batch processes, the proposed method should be extended to address mixed direct and indirect heat recovery networks. Such an extension remains an open issue, particularly with respect to the re-use of HEX units.

# Chapter 4

# CONCLUSIONS & OUTLOOK

## 4.1 Conclusions

The comparative study achieved at the beginning of the PinchBATCH project has shown that the proposed Pinch Analysis (PA) based targeting and design methods perform better (in terms of both heat recovery and cost-effectiveness) than the Omnium Verfahren (OV) and the Permutation Method (PM). The PA based methods feature the unique advantage of providing insight in the problem, but aren't suitable for automated design and optimization.

The identification and the suitable formalization of practice relevant constraints is a prerequisite for the development of automated design methods. Otherwise the provided solutions may turn out to be infeasible or of limited application in practice. The consideration of as many practical constraints as possible also deserves the need to reduce the complexity of the design problem by eliminating at the onset numerous infeasible solutions (e.g. restriction of feasible repipes and resequences of HEXs). Practical constraints have therefore been given due consideration.

The work achieved in the frame of the PinchBATCH project has progressed along 4 complementary lines:

- process specification, practical constraints, preliminary analysis and simplification;
- heuristic methods for targeting and/or simplified design of HR schemes;
- automated synthesis of HR schemes using stochastic optimization methods;

- ♦ specification of batch features and implementation in the PinchLENI / LENIpass software tools.

A short description of the main tools, guidelines and methods developed in these four fields can be found in *Chapter 1, "Executive Summary",* on page 1. Additional comments should be made:

- ♦ the PinchBATCH project provides with a broad base of tools, guidelines, methods, and software specifications, which potential has to be used;
- ♦ although the developed GA based optimization approaches have not been implemented yet, they will likely work. The computing time required to get «optimal» solutions is the most open issue;
- ♦ the ultimate problem of the automated synthesis of mixed direct-indirect heat recovery schemes remains unaddressed. But the development of such a synthesis method appears not to be meaningfull unless the problem of likely schedule variations is analysed and formalized for these additional constraints to be taken into account in the optimization procedure.

## 4.2 Perspectives for Further Work

Several approaches arising from PinchBATCH require further work. The very next steps should be concerned with:

- ♦ the implementation and the validation of the proposed GA based design and optimization approach for indirect batch HR schemes. The validation requires the application on at least 5-10 processes, and sensitivity studies to several parameters to make sure the provided solutions are consistent with expected results;
- ♦ the implementation and the validation of the GA based design and optimization approach for direct batch HENs. A thorough validation procedure (similar to that for the indirect HR schemes) is essential;
- ♦ the implementation of the proposed simplified PA based heuristic method for indirect HR schemes. Optimum HR schemes obtained using the GA approach shall serve as reference;
- ♦ the possible extension of the GA based optimization to mixed direct-indirect HR schemes;
- ♦ the demonstration, on the basis of 2 industrial batch processes, of the overall procedure resulting from the application of the various tools

provided for the preliminary process analysis and simplification, the targeting of the HR modes, the design and optimization, and consideration of rescheduling opportunities, schedule variations, etc.

The following tasks are to be considered in second priority:

- the detailled consideration of schedule variation issues and possible ways to account for these variations at the targeting and design stages;
- the development and validation of a general procedure to address mixed direct-indirect heat integration problems;
- the development of simplified targeting methods for indirect and mixed direct-indirect HR schemes. The validation of these methods shall benefit from reference solutions obtained using the GA based optimization;
- the consideration of hot process water needs at the targeting stage (the GA based optimization should account for this issue at the design stage);
- and finally the implementation into the LENIpass software. The tools and methods for the heat integration of batch processes obviously require to be implemented in a software package to make these suitable for practice. Experience has shown that the associated work should not be underestimated. A development team is necessary, and this task should preferably be assigned to a company specialized in process simulation.

# Chapter 5

# ABREVIATIONS & SUBSCRIPTS

## 5.1 Abreviations

| Abreviation | Meaning |
|---|---|
| BCC | Batch cascade curves |
| CA | Cascade analysis |
| DOF | Degree of freedom |
| EMAT | Minimum approach temperature (=$\Delta T_{min}$) |
| FTVM | Fixed temperature/ variable mass |
| GA | Genetic algorithm |
| HEN | Heat exchanger network |
| HEX | Heat exchanger |
| HR | Heat recovery |
| HRAT | Heat recovery approach temperature |
| HSU | Heat storage unit |
| LSTP | Limiting supply temperature profile |
| MBC | Multiple base cases |
| MER | Maximum heat recovery |

**Table 5-1** List of the abreviations.

| Abreviation | Meaning |
|---|---|
| MHX | Maximum heat exchanges |
| MP | Mathematical Programming |
| OV | Omnium Verfahren |
| PA | Pinch Analysis |
| PM | Permutation Method |
| PO | Post-optimization (in the context of the PM) |
| Sss | Storage sub-system |
| TAM | Time average model |
| TDF | Temperature driving force |
| TES | Thermal energy storage |
| TIAT | Temperature interval approach temperature |
| TS | Time slice |
| TSM | Time slice model |

**Table 5-1** List of the abreviations.

## 5.2 Subscripts

| Subscript | Meaning |
|---|---|
| $i$ | Hot process stream ($i$ = 1 .. $I$) |
| $j$ | Cold process stream ($j$ = 1 .. $J$) |
| $k$ | Heat storage unit ($k$ = 1 .. $K$)<br>Storage sub-system ($k$ = 1 .. $K-1$) |
| $l$ | Time slice ($l$ = 1 .. $L$) |
| $m$ | Hot utility ($m$ = 1 .. $M$) |

**Table 5-2** List of the subscripts.

| Subscript | Meaning |
| --- | --- |
| $n$ | Cold utility ($n$ = 1 .. $N$) |
| $p$ | Process stream ($p$ = 1 .. $P$) |
| $u$ | Utility ($u$ = 1 .. $U$) |

**Table 5-2** List of the subscripts.

# Chapter 6

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# Appendix A

# LITERATURE REVIEW

## A.1 Introduction

This appendix reviews publications which are considered as particularly relevant to the project. It complements the former literature reviews presented in Krummenacher & Favrat (1995), and Krummenacher & Auguste (1997). Each publication is first summarized, followed by a list of comments.

Any classification of papers is difficult and somewhat arbitrary. However, it has been felt usefull to categorize roughly, with respect to the methodology used, into:

- Pinch Analysis based heat integration methods and tools (*Section A.2* on page A-2);
- simplified combinatorial approaches to heat integration, without resorting to Pinch Analysis to provide insight into the problem (*Section A.3* on page A-9);
- HEN design methods based on Mathematical Programming (*Section A.4* on page A-26). The review focuses on the superstructure aspect in the design of continuous HENs, since superstructures are also required for the design of batch HENs using Genetic Algorithms;
- HEN design methods based on Genetic Algorithms (*Section A.5* on page A-34). Reviewed papers address the design of continuous HENs, but valuable experience can extracted for the design of batch HENs too.

# A.2 Pinch Analysis Based Heat Integration

## A.2.1 Wang & Smith (1995)

This paper presents a new approach for analysing the heat integration of batch processes. The time pinch analysis treats time as the primary constraint, while temperature driving forces are treated as secondary constraints - unlike the traditionnal approaches such as the time slice model or the cascade analysis (Kemp & Deakin, 1989), which consider temperature driving forces as the primary constraints. The time pinch analysis assumes that heat is first shifted in time, at the highest temperature level, and then, if a heat surplus still exists, cascaded in temperature. Three types of application are presented (heat integration of batch processes, utility system design, wastewater minimization), of which only the first two are relevant for heat integration purposes.

For time pinch analysis, a new type of composite - the time composite - is introduced. For example, a cold time composite is obtained by plotting $\Delta Q$ of cold process streams versus time; similarly, a hot time composite can be drawn. Unlike temperature composites, time composites can be shifted vertically, i.e. time coordinates are unchanged, while $\Delta Q$ coordinates are arbitrary. Break points on time composites are located at start / stop times of streams, i.e. at the limits of time slices.

### *A.2.1.1 Heat Integration of Batch Processes*

No temperature information is included in the time composites. This means that heat recovery from a hot composite to a cold composite by heat storage implicitely assumes that the constraint of positive temperature driving forces is satisfied.

To make sure that this is the case, given a $\Delta T_{min}$ constraint, the process is divided into (shifted) temperature intervals and a pair of hot / cold time composites is drawn for each temperature interval. This way, the condition of positive temperature driving forces is satisfied, at the expense of a more complicated analysis, because of the temperature interval by temperature interval analysis.

Note that temperature intervals are analysed in the decreasing order of temperature, in order to account for the possibilty of cascading excess heat of a former interval to the next temperature interval. The total heat recovery potential can be targeted, while the indirect heat recovery (and the storage time) is easily identified by plotting the time grand composite. The time grand composite provides insight in the problem of selecting which stream should be rescheduled in order to decrease the requirement for heat storage.

### A.2.1.2 Utility System Design

A utility system has to be optimaly suited to the demand on utility from the process(es). The utility demand can be represented as a cold time composite, while the heat supplied by the utility system (which is constrained by the planned or existing units (steam boilers, etc.)) is represented as a hot time composite. The irreversibility of indirect heat recovery with respect to time is equivalent to assuming single batch (as opposed to repeated batches).

Using the concept of time composites, it is shown that utility systems with an installed capacity smaller than the largest demand in any time period is feasible, if a steam accumulator (which heat capacity can be easily identified on the time composites) is introduced. In this application of time composites, there is no need to care about the temperature constraints, as long as a pair of time composites are drawn for each type of utility.

### A.2.1.3 Comments

The time pinch, which results from replacing temperature by time and heat rate by heat, demonstrates once again that the concept of pinch is very general indeed.

Although basically quite simple and providing good insight in the problem due to its graphical representation, the time pinch analysis still suffers from several limtations:

- the introduction of temperature constraints for a real process generally leads to a large number time composites, since one pair of time composites is required for each temperature interval, a representation which is not easier to handle and undestand than the temperature composites for each time-slice when priority is given to direct heat recovery. An overall assessment of the required heat storage units is not possible - combining the information from the various temperature intervals into a single comprehensive representation is hardly possible. Once again, an overall representation, able to easily account and understand both time and temperature constraints is missing. Rather, one has to work with a set of dedicated representations providing insight in a particular aspect of the problem;

- as with the cascade analysis, a single $\Delta T_{min}$ for all stream matches is required when accounting for the temperature constraints. This is an intrinsic limitation of time pinch analysis;
- the time pinch analysis provides (energy) targets for direct and indirect heat recovery (for a given $\Delta T_{min}$). It is rather a preliminary analysis tool to be used to make high level decisions such as process / scheduling changes. But, it is likely not suitable for supertargeting and design purposes, because of the too crude assumptions behind the methodology;
- with respect to the feasibility of indirect heat recovery, the case of repeated batches is unfortunately overlooked;
- although easier identification of rescheduling opportunities using the new graphical representations is advocated, it is still difficult to efficiently apply the technique to real industrial processes, since in general any indirect heat recovery pocket results from the combined effect of several streams, and also from the fact that a given stream often contributes to several pockets, hence rescheduling it to decrease a particular pocket shall have side-effects on the other pockets;
- modifying the cascade analysis so that heat is shifted in time before being cascaded in temperature, would provide similar results.

### A.2.2 Sadr-Kazemi & Polley (1996)

A heat integration methodology of batch plants based on heat storage systems has been proposed by Sadr-Kazemi & Polley (1996). Unlike a general trend to set the priority to direct heat exchanges, this paper deliberately considers the indirect heat recovery alternative. The reason for favouring heat storage rather than direct heat recovery is the fact that the batch schedules are often not fixed and are subject to both stochastic and deterministic variations. If process streams are integrated through direct heat exchanges, schedule variations might penalize the heat recovery and have detrimental effects on the plant capacity. Heat storage provides the batch plants with the desired flexibility by decoupling the hot streams from the cold streams with respect to their actual schedule.

Following Gremouti (1991), these authors also recommend the use of external pre-heating (when charging) and post-cooling (when discharging), instead of using the vessel jacket for this task (less temperature cycling of the heavy jacketed reactor, higher heat transfer coefficient and shorter heating and cooling time, increased heat recovery potential due to steady state conditions for the heat transfer fluid).

Depending on whether the external heating / cooling strategy can be applied or not, two different storage systems / operating modes are considered:

- steady state heat storage systems, for processes where external heating / cooling strategy can be used (i.e. without large temperature cycling of the reactor vessel);
- unsteady state heat storage systems, for cases where in-vessel heating / cooling can't be avoided.

Steady state heat storage means constant operating temperatures of the storage tanks, while unsteady state occurs when these operating temperatures are allowed to vary continuously as a function of the task in progress (although lower and upper temperature bounds are specified for each tank).

### A.2.2.1 Steady State Heat Storage Systems

Steady state heat storage systems are designed according to the following procedure:

1. calculate the "total duty composites" of the process (in heat rather than in heat rate). These composites are actually equivalent to TAM (energy) composites;
2. select a $\Delta T_{min}$ between composites;
3. on the composites, identify the scope for heat recovery as given by the overlap of composites curves (defined by the selected $\Delta T_{min}$) and choose which streams are actually going to transfer this amount of heat recovery (generally, the number of streams involved should be minimized);
4. calculate the duty composites for the selected set of streams;
5. select the number of storage tanks and their operating temperatures, accounting for the trade-off effects between increasing the number of

storage tanks (to increase their temperature span and hence decrease their overall storage capacity), or selecting the minimum number of storage tanks (at the expense of increased storage capacitity and larger heat exchange area whenever the temperature driving forces are reduced). The storage temperatures are defined according to the supply temperature of the streams to be integrated;

6. given the driving force from hot streams to storage tanks, and storage tanks to cold streams, the HEXs are sized and costed;
7. knowing the operating temperature level of each storage tank, the heat load to be stored and their schedule, the minimum capacity of the tanks are calculated;
8. it is then analysed if the size of the tanks and the heat storage fluid inventory could be reduced by modifying the operating schedule, resulting in capital cost savings;
9. the operating temperature of the storage tanks can be varied to analyse other heat storage schemes;
10. the trade-off between capital costs and energy costs can be explored by varying the $\Delta T_{min}$ (iterate steps 3 to 9).

#### A.2.2.2 Unsteady State Heat Storage Systems

If safety or process considerations prevent the feed / product streams to be pre-heated / post-cooled externally during charging / discharging, unsteady state heat storage is considered. It is stated that in this mode of operation, the minimum number of storage tanks is one (instead of two in steady state).

At the root are the heating and cooling curves of batch reactors: while the inlet temperature of the heat transfer fluid is maintained constant during the whole heating / cooling phases, its oulet temperature constinuously varies (i.e. increasing during heating, decreasing while cooling), and the inlet-outlet temperature difference and the corresponding heat rate vary accordingly.

It is argued that it is no longer possible to assume that the tanks operate at constant temperatures and that it is better to allow the temperatures of the tanks to vary.

General schemes for the "heat absorption leg" and the "heat rejection leg" are proposed. In addition to storage tanks and heat exchangers, these schemes also include utility heaters and coolers, which increase the flexibility of the system. The strategy to operate such schemes is based on several test conditions (of the type «temperature > $T_j$ ?») to select the tank where to return the heat transfer fluid and to decide whether it should be first cooled or heated. How these temperature set point values (design variables) are set is not described.

In addition, different aspects of unsteady state heat transfer are analysed: various operating scenarios, their influence on the heating and cooling time of batch reactors.

### A.2.2.3 Comments

Like most of the heat integration methodologies proposed so far, this approach falls in the category of "either-or" (as opposed to "both" direct and indirect heat recovery).

The procedure proposed for the design of steady state heat storage systems is in many respects similar to the one proposed by Krummenacher & Auguste (1997), which has been derived from Krummenacher & Favrat (1995) for the particular case of heat integration being exclusively achieved by heat storage (100% indirect heat recovery).

The choice of the number of storage tanks and of their operating temperature is subject to the same trade-off effects. To achieve a specified level of heat recovery at least overall annual costs, the choice of the streams to be integrated is critical. Although it is sensible to minimize their number, do not sacrifice temperature driving force too much. The required number of heat storage tanks and their size depend on the schedule of the selected streams; therefore, select streams sets featuring short delays between heat supply and heat use (high simultaneity factor). But do not forget to account for the duration of streams selected; long duration are advantageous, since it decreases the size (heat rate) of the corresponding HEXs.

The proposed procedure is worth some remarks:

- although simple in essence, the procedure hides actually both combinatorial and parametric optimization difficulties, and ways to solve these are not explained;
- to arrive at cost-optimum solutions, numerous configurations need to be actually designed and evaluated. Almost no supertargeting (i.e. pre-optimisation with respect to economics) is performed. User input is

required for selecting the configurations and choosing the value of their paramaters (to compare with heat integration of continuous processes, the the decision of the user to match streams and select the heat rate during HEN design). The procedure is time-consuming and, whenever possible, a supertargeting approach would be required. Fundamental insight in the trade-off effects has to be developed, from which new tools for their quantitative assessment are expected to emerge;

- depending on the shape of "total duty composites" and the available driving forces, the room to manoeuvre might be quite limited, as opposed to the process used to demonstrate the design procedure of steady state heat storage system;
- a systematic methodology for process rescheduling is not described; rather, simple heuristic rules such as synchronization of extraction and feed in the storage tanks are proposed. Given a design, it would also be interesting to provide the user with a method for assessing "schedule margin" within which a heat recovery penalty is not incurred;

As far as unsteady state heat storage systems are concerned, the following comments should be made:

- the reason why the steady state mode (i.e. control of the heat transfer fluid return temperature to maintain the tank temperature constant) cannot (or should not) be envisaged is not explained. Variable outlet temperature could be managed by switching from a tank to another one during the course of the reactor heating or cooling;
- more importantly, the heat recovery issues are completely overlooked. The way the various strategies (e.g. the non-isothermal mixing, the possible return of the heat transfer fluid in the same tank) affects the heat recovery is not described;
- how can both steady and unsteady state systems be combined, since both are likely to be needed for the same batch plant ?

# A.3 Combinatorial Design Methods

## A.3.1 Introduction

The two main combinatorial methods for designing heat integration schemes for batch processes, namely the Permutation Method (PM) and the Omnium Verfahren (OV), have already been reviewed in Krummenacher & Auguste (1997).

Both methods have been further developed, and are therefore worth an up-to-date analysis. The recently improved PM deserves an extended analysis, since it leads to a major new approach to the heat integration of batch processes.

## A.3.2 The Permutation Method

The Permutation Method (PM), first presented by Stoltze *et al.* (1992, 1995), has been further improved and extended (Mikkelsen, 1998; Mikkelsen *et al.*, 1998).

The basic assumption behind the PM is that the heat recovery is exclusively achieved by indirect heat exchanges using heat storage. Although generally more expensive, this mode of heat integration is preferred as it provides more flexibility and increased operability, which are highly desired features of batch plants.

In addition, it has been argued that the combinatorial complexity is much lower compared to the problem of designing batch HENs for direct heat recovery, allowing for "exhaustive" searches of the most profitable configurations within reasonable computing times to be performed. It also results in fewer heat exchanger units.

As presented, the PM also assumes:

- "fixed temperature - variable mass" (FTVM) heat storage units;
- repeated batch operation and counter-current heat exchanges.

The design methodology (Mikkelsen, 1998; Mikkelsen *et al.*, 1998) involves actually three steps: 1) determination of the pinch using TAM composites;

2) simplified combinatorial search (PM); 3) post-optimization (PO) of the most interesting configurations resulting from step 2.

### A.3.2.1 Step 1: TAM Composites and Pinch

The TAM composites are calculated to identify the pinch point, the related utility targets, and the heat recovery target for a chosen $\Delta T_{min}$. If needed, streams are splitted at the pinch, in order for the heat recovery target to be achievable. Identifying the pinch temperature is also useful in case of soft streams (i.e. a stream which target temperature is allowed to vary within two limits), or heat recovery streams (i.e streams which are not process streams and hence not compulsory - called free utility in the context of the PM).

### A.3.2.2 Step 2: Simplified Combinatorial Search

After splitting process streams at pinch whenever needed, a combinatorial search for the most "profitable" configurations (streams - heat storage matches) is performed. During this search, "all possible" configurations are generated by permutation of n storage temperatures (out of the discrete set of possible storage temperatures) and, for each storage configuration, permutation of s streams (out of the total number of process streams) to be integrated with the n storage tanks. «The basic idea is to discover the optimal set of store temperatures and process streams to be integrated by permutation of both store temperatures and process streams».

The number of configurations to evaluate is actually reduced by criterias of two kinds: 1) simple heuristic rules and 2) estimating functions.

The simple heuristic rules include:

- the possible discrete temperature levels of heat storages are generated according to the supply and target temperatures of process streams, corrected for the minimum temperature difference requirements (i.e. half the $\Delta T_{min}$ selected on TAM composites). Note that the set of operating temperatures can also be specified by the user;
- during the search, each process stream is matched to the pair of storage units which operating temperatures are the closest to its supply and target temperatures. This rule tends to minimize the number of HEXs by requiring only one HEX for each stream. However, in the absence of any other suitable storage unit, a stream which only partly "fits into" the

temperature range of a pair of heat storages shall only be partly integrated in order to maintain feasible temperature driving force. The remaining part of the stream shall be met by utility;

- mass imbalances existing in heat storages after a batch cycle are leveled off first by mixing between storages. Remaining imbalances are finally corrected using utilities;
- lower and upper bounds for the number of process streams to integrate with heat storages can be specified by the user allowing for some kind of control on the search procedure and hence on the computing time.

In addition to the above heuristics, three estimating functions have been included. Their aim is to identify unpromising sets of configurations as soon as possible in order to skip further calculation of these configurations (i.e. save a significant amount of computational time needed for permutation of the streams to be integrated using only a limited amount of computational work).

Estimated are the heat recovery potential, the cost of equipements and the objective function. These estimates cannot guarantee true lower bounds (for minimization) or upper bounds (when maximizing). However, used in a hierarchical manner, they provide the search algorithm with some degree of intelligence.

The "most profitable" configuration is assessed with respect to one (or more) of the following possible objective functions:

- the payback period of investment for the heat recovery system (to be minimized);
- the net present value of savings NPVs (to be maximized);
- the ratio between savings and payback period (to be maximized);
- the amount of heat recovery (to be maximized).

Inherent to the procedure is the ability to provide the user with a ranked list of the m "best configurations" (instead of just supplying "the best one").

The optimization can handle both grassroot and retrofit design. The retrofit design capability is restricted to the case where utility heat exchangers already exist for all process streams and therefore their costs, unlike grassroot design, should not be included in the investment costs.

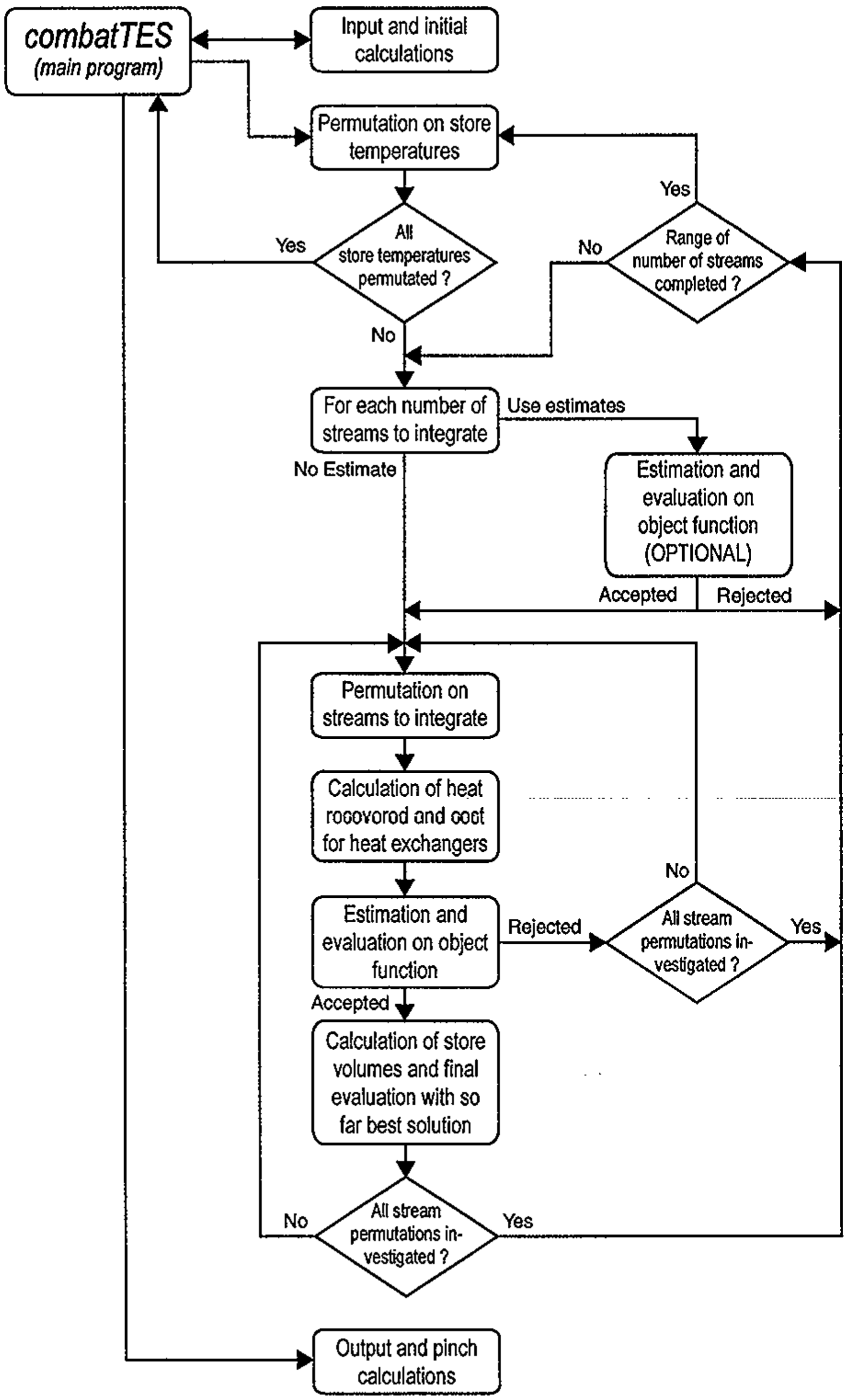


**Figure A-1** Simplified flowsheet of the software tool «CombatTES» (Mikkelsen, 1998).

The search is performed for a specified number of storage units. In order to find the "overall optimum heat integration configuration", the user should begin with a low number of heat storage tanks (at least 2 units) and then increment the number of tanks one at a time. It is sensibly assumed that, if the value of the objective function for the optimum configuration ceases to improve after the number of storage units has been increased by one unit, the "overall optimum configuration" has been identified.

In practice, the comparison of "optimum configurations" for two successive numbers of storage units is only meaningful after a post-optimization of these configurations has been performed. This is so because the PO has demonstrated large improvement potential in some cases.

Repetitive search tasks of step 2 are actually performed by a software tool named «CombatTES», which simplified flowsheet is depicted in *Figure A-1*. CombatTES offers numerous options, during the specification of the process stream table and the techno-economic data, as well as for running the search (e.g. process streams and free streams, streamwise $\Delta T_{min}$ specification, various energy and monetary units, several cost functions for HEX and storage units with area and capacity limits, possibility to modify cost factors of streams to account for the reuse of heat exchangers, the way the heat storages are sized - designed for including or excluding imbalances over a batch cycle, etc.).

These options make the method suitable for a wide range of process and project conditions, and allow for a better adaptation to real problems. However, their selection requires skill and experience from the user.

#### A.3.2.3 Step 3: Post-optimisation

The former step (step 2) involves the discretization of many variables; the "exhautive" search for "the best configuration" actually searches at discrete locations (something like a grid) in the space of solutions. It can be viewed as a structural optimization, without any optimization of continuous parameters (e.g. operating temperature of storage tanks, amount of heat recovered from each stream). Resorting to simple heuristics may overlook potentially better solutions. There is therefore scope for further improvement (called «post-optimisation» (PO) in this context) to be performed as step 3. The PO can involve one or more of the following aspects:

1. fine tuning of the discretely optimized storage temperatures;

2. modify the way (in particular the schedule) the required utility loads are supplied to process streams;
3. adjusting the cut-off temperature of integrated streams;
4. optimization of the schedule of mixing between storages for rebalancing (to reduce the required storage capacities);
5. relaxation of stream-store matching rule;
6. relaxation of the fixed storage temperature constraint during a batch cycle.

These techniques stem from systematically revisiting the simple heuristics and identifying opportunities for improvements. The principle is to reduce the number and/or the size of HEXs (e.g. using a more flexible configuration), and/or decrease the heat storage capacities.

Note that these relaxing rules can be compared to the loop and path strategy applied to continuous HENs. However, the above techniques are "fuzzy" and much less formalized and systematic.

With respect to the PO technique 2: a utility HEX supplying heat during rebalancing of storage mass is substituted by pre-heating a storage stream during its use. Instead of storing utility heat, it is supplied directly when needed (yet on the storage stream and not directly on the process stream). In principle, the storage capacity can be decreased, while the number of HEX units and the required HEX area are also influenced. In practice, generaly complex trade-off effects come into play; the benefits depend on:

- the opportunity for rebalancing during a period of time and at a low mass flowrate, so that over-capacities of storage are not required;
- whether the required utility heat can be supplied to one process stream only or need to be splitted between several process streams, eventually requiring more HEX units;
- the possible existence of a utility heater downstream on the process stream(s) to which utility should be supplied by application of PO technique 2;
- the various temperature driving forces of the HEXs involved.

The different PO techniques obviously interact with each other, and should ideally be optimized simultaneously. The complexity of the trade-off effects makes this very tedious, if ever possible, to do so in practice, except for simple processes. «The techniques have been investigated by formulation and optimization in EES (Engineering Equation Solver, Klein & Alvarado, 1992-1996). Even in such an environment, the PO procedure is tedious and can be regarded as evolutionary in the sense that different techniques are combined according to trial and error. The optimization carried out by EES cannot guarantee global optimum for the usual problems, and involves initial guesses. The success of optimization relies on how good and qualified the initial guesses are».

The improvement potential using PO is reported to span from 3% up to 25% in the case of a brewery, depending on the number of process streams that were to be heat integrated. It is argued that the potential is expected to be low when only part of the process streams are required to be integrated, as there are a large number of possible configurations (i.e. ways to select the number of streams to integrate among the total number of streams), giving a large choice to select the best one. While this choice becomes more and more restricted as the number of streams to be integrated tends towards the number of process streams. Large improvement potential is expected in this case.

In addition, there is no guarantee that the "optimal solution" has been found; the achieved improvement depends on the user's skill.

To by-pass this problem and hopefully automate the PO step, superstructures embeding all the possibly beneficial alternatives included in the above techniques are presented. The corresponding mathematical programming model and it resolution using MINLP solvers remain to be developed.

#### *A.3.2.4 Additionnal Work*

Apart from developing the 3-steps design procedure of thermal-energy storage (TES) systems, sensitivity analysis and dynamic simulation have been performed, in order to ascertain the operability and the flexibility of such TES systems.

The sensitivity of TES to various variables (temperature of heat storages, and starting temperature of matched process streams) in off-design situations has been considered. Their propagation has been simulated under various control strategies and corrective actions. The prioritary control of the target temperature of process streams turned out to be a better strategy than controlling the target temperature of storage streams to maintain storages at fixed temperature. The TES systems actually allow for decoupling (or weak coupling) between integrated streams.

TES systems are found to be stable and able to cope with both large off-schedule situations of random character and rescheduling of processes without compromising the degree of heat recovery.

Further work is also suggested, in particular:

- further refinement of design heuristics of PM (particularly for situations where PO identifies large improvement potential);
- improvement of the estimating functions;
- math. programming formulation of the superstructures for PO;
- general formulation of "off-schedule margin" and "rescheduling margin" for a given TES system.

### *A.3.2.5 Comments*

The TES systems and the design procedure based on PM are an original and valuable approach to the heat integration of batch processes. High flexility, operability, and tolerance to off-design situations are major advantages, for which higher investment costs can be accomodated. Mikkelsen (1998) has laid firm foundations and proposed skilled solutions for cost-effective TES systems.

Whatever practice oriented, the proposed 3-steps procedure still leaves the design engineer with the following difficulties:

1. the problem of how to identify the optimum $\Delta T_{min}$ before carrying out the procedure remains unadressed. The complete procedure could of course be performed for various $\Delta T_{min}$, allowing to identify the optimum pinch. A "targeting before design" solution would be preferred to this rather time-consuming approach. It could be argued that the "optimal region" be quite flat around the optimum $\Delta T_{min}$ so that "small" deviation of a few °C would not matter. But there is neither experimental nor theoritical evidence that it is actually the case. Unlike continuous processes, batch processes show largely different running hours/year values and hence make the assessement of a reasonable $\Delta T_{min}$ difficult;
2. within the PM (i.e. during step 2), configurations are continuously compared to the "best configuration" found up to the time of comparison; the compared configurations can of course show completely different structures. Knowing that further improvement of a solution by PO can be as high as 25% (this value depends very likely on the configuration), this

makes the comparison, within the PM, of configurations showing a difference of, say, half this value (i.e. 12%) quite questionable. There are certainly a large number of configurations for which little can be said before the PO step has been performed. The many PO techniques aimed at improving the configuration selected according to the simplified PM heuristics are actually not only "fine adjustments";

3. the procedure is quite flexible in that it provides the user with many options. Skill and experience is required to actually take advantage of these. There is still place for trial and error, as few firm guidelines and almost no representation that would provide insight in the problem are proposed or used;
4. owing to the lack of insight in the problem, the relation between the minimum number of storages and the heat recovery potential is not addressed. The effect of stream scheduling on the minimum number of storages is overlooked. In this respect, the brewery case study might not be considered as typical, as large temperature driving forces are available;
5. the reuse of HEXs is supported by CombatTES, but no systematic method to account for it and optimize it has been proposed;
6. in many batch plants (e.g.breweries), large quantities of process hot water, or hot water for cleaning purposes, are required. The "free scheduling" and "storable" properties of such process streams cannot (or at lest has not) been taken into account;
7. how does the heat integration using TES compare to direct heat exchanges integration is not mentionned. What is the price to pay for flexibility ?
8. what would happen if the storage temperature required by the process be not compatible with water (i.e. much larger than 100°C) ?
9. the search for a minimum number of HEXs may be particularly supported by their (assumed) high initial costs.

In conclusion, the approach of using TES systems is very valuable, but the proposed methodology to design such systems is still quite complicated. The detailled work performed and the variety of discovered trade-off still appear as numerous pieces of a puzzle which image is not yet known. In particular, the user is missing tools providing insight in the problem.

### A.3.3 The Omnium Verfahren

Shortly after being published (Hellwig & Thöne, 1994), the Omnium Verfahren (OV) has been the subject of a detailled comparison with a Pinch Analysis (PA) based approach (Uhlenbruck, 1995). The comparison has actually been performed for both continuous and batch processes. Then, after identifying the intrinsic limitations of the original OV, solutions for improving its performances were suggested. A recent paper (Uhlenbruck & Vogel, 1999) presents the strategy to improve the degree of heat recovery which has been developed in Uhlenbruck (1995); in addition, this paper provides with statistical values for the maximum degree of heat recovery using the OV.

As a short reminder, the OV has originaly been developed to provide the user with an automated search of the "best" heat exchanger network, i.e. the one showing the highest global heat recovery potential. The processes to be heat integrated are most generally time dependant processes (e.g. several processes operated in small to middle size companies, e.g. dairies, etc.), not strictly batch process streams. The OV assumes exclusive hot stream-cold stream matches, that is once a heat exchanger is placed between a hot and a cold stream, neither the hot, nor the related cold stream are allowed to further exchange heat with any other streams (be it simultaneously, for the possibly remaining unused heat, or at another time period, while one of the stream pair does not exist). In other words, there may exist at the most one internal heat exchanger on any process streams (the rule only applies to internal heat exchanger, not to the external heaters and coolers).

The problem is best represented in the form of matrix in which the hot streams are organised in columns, while the cold streams are entered in rows. Each element of the matrix (i.e. the possible match of a cold stream with a hot stream) is assigned the maximum amount of heat that may be recovered if the corresponding match is selected. Then the combination of independant matches (i.e. selection of at the most one element in each row and each column) giving the highest total heat recovery is searched for. The selected matches define the process-to-process HEN.

Several reasons for considering exclusive matches can be mentionned. Firstly, exclusive matches provide simple, manageable HENs, which will more likely be accepted in industry than complicated HENs. Secondly, it is assumed that exclusive matches shall limit the HENs to the most cost-effective HEXs. Thirdly and most importantly, this assumption allows to express the optimization of the heat integration as an allocation problem (Zuordnungsproblem) and to solve the problem using a modified version of the Ungarian Algorithm. In the OV, the economics is accounted for by the specification of a $\Delta T_{min}$ value for heat exchanges between any hot stream-cold stream match.

To compare with the OV, Uhlenbruck has also designed HENs by making use of basic concepts of Pinch Analysis (PA). A quantitative comparison has focused on the energy targets and the number of HEX units (without any cost calculation); other benefits and drawbacks of rather qualitative nature have been highlighted.

#### A.3.3.1 Comparison on the Basis of Continuous Processes

Although the OV has been developed for time dependant processes, it can be applied to continuous processes as well. HENs for 3 processes (with 4, 19, and 53 process streams, respectively) have been designed with both the OV and the PA approach. Only basic tools of the PA such as the composites curves, the problem table algorithm (grand composite), the energy targets for a selected $\Delta T_{min}$, the pinch desigh method and the relaxation using loops and paths were used. The path relaxation was also applied to OV HENs, whenever sensible.

The main conclusions for these test cases are:

- all OV HENs have significantly higher utility consumptions than MER targets. Since the process pinch is not taken into account, the OV HENs generally violate the pinch rules, i.e. heat is often transfered across the pinch, hot utility is used below the pinch, or cold utility is used above the pinch;
- OV do not necessarily lead to HENs with less HEX units; more utility HEXs compensate for less process-to-process HEXs;
- the design of OV HENs is automated, hence easier than PA HENs, particularly for processes with a large number of streams;
- the PA approach provides the design engineer with much more information than "simply" the HEN design, e.g. insight in the process such as the knowledge of the pinch or the minimum exergy level of utilities. A theorical analysis of the process cannot be made using the OV;

- on the whole, the OV is not suited for the design of continuous HENs.

### A.3.3.2 Comparison on the Basis of Batch Processes

Three batch processes have been considered, with 4, 7 and 4 streams, respectively. The comparison of the OV and PA HENs has been achieved on the basis of direct heat exchanges only.

For the design of batch HENs according to the PA approach, the Time Slice Model (TSM) and the Cascade Analysis (CA) (Kemp & Deakin, 1989) have been used. A single $\Delta T_{min}$ for all time slices has been assumed (actually imposed by the CA). The design strategy used for the PA approach consists of the following steps:

1. identification of the time slices, calculation of the corresponding heat cascades for the specified $\Delta T_{min}$;
2. identification of the pinch temperature locus and the energy targets;
3. design of a MER HEN for each time slice, i.e a HEN achieving the energy targets if this continuous sub-process is considered for itself;
4. merging (superposition) of the various HENs into one single "overall HEN". This HEN achieving the overall maximum direct heat exchanges is named a MHX HEN;
5. relaxation of the MHX HEN to improve its cost-efficiency, in a quite similar way to continuous HENs.

The comparison has resulted in the following conclusions:

- the design of PA MHX HENs is significantly more time-consuming (yet not particularly difficult);
- the relaxation of PA MHX HENs is not a straighforward task and is actually the critical step in the PA approach;
- with the relaxation, the PA MHX HENs have evolved in the "direction" of OV HENs; the relaxed PA HENs lie somewhere between the PA MHX HENs and the OV HENs, and are found to be structurally compatible with the later. This means that removing one or more HEXs from the relaxed PA HENs leads to the corresponding OV HEN;
- as the OV HENs are much more easily designed, the former observation leads to the idea of resorting to the OV for developing an initial HEN, which can further be improved by including additional HEXs;

- the heat recovery of the OV HENs is often significantly lower than both the PA MHX HENs and the relaxed PA HENs. This intrinsically results from the OV requiring exclusive matches;
- heat storage opportunities are not addressed by the OV, while the PA approach allows such an assessment and also provides the user with additional insight in the process (e.g. the proven "target before design" strategy, etc.).

### *A.3.3.3 Suggested Improvements of the Omnium Verfahren*

The comparison of OV versus PA HENs for the design of batch HENs has shown advantages and drawbacks of both methods. The PA is essential for a preliminary process analysis, as well as for the definition of targets (here, mainly energy targets). The OV is the preferred method for automatically designing an initial HEN solution, which remains to be improved (with respect to heat recovery).

- To bypass the limitation deriving from the assumption of exclusive matches, a first proposal is to split streams in parts of equivalent heat rate, either in temperature (serial split - lead to serially connected HEXs) or in heat capacity flowrate (parallel split - leads to parallel connected HEXs). Since any process stream is splitted into several sub-streams, the application of OV to the matrix of sub-streams now allows several matches for each process stream (while the assumption of exclusive matches still holds at the level of each sub-stream). Making sub-streams equivalent in heat rate allows to place "tick-off" matches, i.e the remaining heat rate after a match has been selected is zero. The finer the subdivision of streams (i.e. the smaller the heat rate elements), the larger the achieved heat recovery of the OV HENs. The so designed HENs consist of many small HEXs which should first be grouped together to obtain more simple HEN structures. It is claimed that if the subdivision of streams is sufficiently fine, the MER targets can be reached. The selection of a sensible elementary heat rate is a way to control the degree of heat recovery - the aim is not necessarily to reach the MER target.
- A less complex proposal to bypass the exclusive matches limitation is to repeatedly apply the OV (this is the method actually described in Uhlenbruck & Vogel, 1999): after a first OV run, the remaining streams or part of streams are listed and a corresponding matrix of (remaining) maximum heat recovery is calculated. The OV is run to find further

matches, which are then added to the matches identified during the first OV run. If needed or still possible, a third OV run can be applied on the remaining matrix after the second run, etc. It is claimed that using this procedure, the OV HENs move towards and actually reach the relaxed PA HENs (at least for the three batch test processes considered)

- Another proposal addresses the problem of including indirect heat recovery (using heat storage) in the OV. The principle is to first exhaust the direct heat exchanges opportunities (i.e. to repeatly run the OV on the remaining heat matrix, as just described, until the remaining (direct heat recovery) matrix elements are all 0), then to recalculate the same matrix without accounting for time schedule (i.e. calculating the maximum possible heat recovery only on the basis of the temperature, not additionaly requiring simultaneity of streams). Note that $\Delta T_{min}$ for heat storage can be selected independantly of the $\Delta T_{min}$ used for direct heat recovery. The OV is then run on this remaining matrix (remaining heat storage matrix). If needed - whenever non-zero elements still exist in the remaining heat storage matrix - the OV can be repeated. For the test cases, the MER targets are achieved, but this result cannot be generalized.
- Arguing that heat cannot be stored over a temperature range but rather at a fixed temperature level (inspired by Kemp & Deakin, 1989), a procedure to identify the optimum temperature level for heat storage is proposed. Since an opportunity for heat storage has been identified using the former proposal, this procedure does not require anymore for exclusive matches for indirect heat recovery: all remaining hot stream contributions (and remaining cold stream contributions, respectively) are added taking into account their temperature level. The optimal temperature level is the one that maximize the usable heat recovery.
- Finally, it is suggested to use the above procedure to first define the optimum storage temperature level for each possible match of the remaining heat storage matrix, to calculate the heat that may be transfered by each match at the corresponding storage temperature level, and run the OV on this matrix.

#### *A.3.3.4 Comments*

Uhlenbruck (1995) provides with numerous test cases and detailled OV versus Pinch comparisons with respect to energy recovery (energy targets) and number of units. The suggested improvements open new perspectives with the OV; as presented, these improvements focus mainly on energy recovery, not on economics (this holds for Uhlenbruck & Vogel (1999), too).

The following comments should be made:

1. neither heat exchange areas nor costs (capital as well as energy costs) are actually calculated and compared, resulting in an incomplete picture. If these parameters were taken into account, the OV might prove even less attractive, at least when applied to maximize the overall heat recovery. Some of the HEXs selected by the OV tend to have large heat duty with small temperature driving forces, leading to very large area and unattractive economics. The HENs designed with pinch usually make much better use of available temperature driving forces as indicated by the composites curves (still depending on the experience of the designer);
2. with respect to the economically optimum heat recovery, the fundamental role of supertargeting (i.e. economic pre-optimisation) has not been taken into account. As long as the supertargeting models are accurate enough, there is no reason to believe that placed heat exchanger are not economical and should be relaxed. If this is the case, than supertargeting shoud be questionned.
3. without any costs consideration, the degree of relaxation to be applied and when to stop simplifying the PA HEN is very questionnable. The optimum degree of relaxation is a question all about economics;
4. as already mentionned, the relaxation of the PA MHX HENs is not straightforward, as one has to keep in mind the time variable during this operation. It is also important to note that for the second and the third processes, the relaxation strategy do not only resort to loop & paths, but involves some tricky ideas how to reuse HEXs across more time slices. In fact, as applied, the relaxation has changed the HEN structure (e.g. HEXs in parallel on a stream have been changed to serially connected HEXs). It can be viewed as an attempt to account for possible HEX reuse (involving structural changes whenever needed), an aspect that has not been considered during the design of individual MER HENs (for each time slice in isolation) - as opposed to a simultaneous design of the various time slice HENs encountered in MBC design. For processes with a large number of streams, such relaxation tricks with significant structural modifications are expected to become impossible to derive by hand;
5. it is claimed that the OV HENs should prove more attractive with respect to economics, since they are made of a restricted number of process HEX

selected because of their large heat recovery potential. This statement is actually not well founded, since the various costs are not calculated. In addition, matches selected on this basis are not necessarily cost-effective if the temperature driving forces are not accounted for;

6. the fact that the structure of relaxed PA HENs is compatible with the one of the OV HENs might be explained by the three processes having a small number of streams (it is yet unclear whether the knowledge of the OV HEN has not biased (implicitly or explicitly) the relaxation procedure by suggesting "tricks" that would otherwise not have been found or selected). However, this feature should not be expected from processes with larger numbers of streams within each time slice: the number of structurally different HENs increases likewise and the probability that a OV HEN and the corresponding PA HEN have the same structure decreases;

7. although the three batch test processes allow to draw general trends, the extent to which the OV HENs actually deviate from the PA HENs depends on the process: number of streams, ability to form independant sub-systems, the relative heat capacity flowrates, etc. From this perspective, the three analysed processes might not be considered as typical batch processes. The process including 7 process streams of quite similar heat capacity flowrate is expected to favor the OV since stream splitting is not required;

8. in any case, an external iteration loop on the $\Delta T_{min}$ is required for an economic optimization. Imposing a single $\Delta T_{min}$ for all matches is questionnable. This has likely not been a problem for the test processes so far, because of the simple structure of the HENs and the fact that major matches begin (or are present) at the pinch, i.e. where the PA HEXs also have $\Delta Tmin$ . But this is not true for matches placed away from the pinch, for which the available driving forces are much larger than $\Delta T_{min}$;

9. in principle, the same solution algorithm could be applied with another objective function. In particular, it might be possible to directly minimize the annual costs (i.e. maximize the benefits from heat recovery matches). In this case, the optimum heat rate of each match should be individually calculated by minimizing the annual cost. In this case, the $\Delta T_{min}$ would be match-dependant and be actually the optimization variable of each match heat rate. The limitation of exclusive matches could be bypassed by a repeated use of the OV. This approach has some similarities with the Combinet method (Mikkelsen & Qvale, 1997);

**10.** the original OV cannot be used to design balanced HENs, i.e. cases where utility HEXs are not necessarily placed at the end (target) side of streams, but rather are incorporated at intermediate temperatures. In fact, it is not possible to specify a 100 % heat balance based on exclusive matches (even when applied iteratively on remaining heat, as possibly inadequate decision where made during preceeding steps). The only solution approach would be a fine subdivision of all streams (including utility streams) into sub-streams of equivalent heat rate;

**11.** the procedure of splitting streams in many sub-streams of equal heat rate can be viewed as a simultaneous, global optimization approach to the design of HENs;

**12.** the suggestion for applying the OV iteratively on remaining heat recovery matrices has to be considered as a sequence of partial sub-optimizations, which in general miss the global optimum. Experience is lacking on the maximum level of heat recovery attainable with this procedure (i.e. where the OV HENs stops to improve). In particular, there is no reason to believe that it will "cross" the PA HENs - it could also stop before this level of economic optimum heat recovery is reached. This procedure relaxes (smoothes) the limitation set by assuming exclusive matches;

**13.** for both the OV and PA HENs, the reuse of HEXs across time slices is limited to the *conventional* type. Possibilities for *resequence* or *repipe* type (Jones, 1991; Krummenacher & Favrat, 1995) are not taken into account. Could this be done ? Could the OV be applied to each time slice accounting simultaneously for the other time slices ? Could the pinch be accounted for ? How to design HENs structures compatible with PA MHX HENs ? Processes which HENs have different structural alternatives remain to be analysed;

**14.** with respect to the proposal to account for heat storage in the OV, note that it is not intrinsically necessary to first exhaust the direct heat recovery potential.

# A.4
# HEN Design Methods Based on Mathematical Programming

## A.4.1
## Motivation

The design of batch HENs based on pinch design methods is time-consuming and the relaxation is tedious (Krummenacher & Favrat, 1995; Uhlenbruck, 1995). It differs from the design of continuous HENs in several ways (e.g. simultaneous development of several HENs - one for each time slice - which should as much as possible be structurally compatible with each other in order to maximize the reuse of HEXs across time slices). Automated design methods based on Mathematical Programming could possibly be developed for such batch HENs. However, two sources of difficulties are to be expected:

- structural difficulties might even be higher for batch HENs than for continuous HENs;
- the reuse of heat exchanger across time slices and the need to account for various other costs contributions (piping, valving, by-pass to make this reuse possible).

Actually, the motivation to analyse the Mathcmatical Programming methods mainly concerns the HEN superstructures that have been proposed so far for continuous HENs. The following review does not pretend to be exhaustive, and is rather intended to provide some fundamentals. Significant contributions, published after 1991, are not analysed below. Several among them are actually mixed approaches, taking advantages of both the Pinch Analysis and the Mathematical Programming approaches (e.g. Zhu, 1995; Zhu *et al.*, 1995; Briones & Kokossis, 1999).

## A.4.2
## Floudas (1995)

In his book entitled «Nonlinear and Mixed-Integer Optimization», Floudas provides an exhaustive review of mathematical programming methods for HEN design (up to about 1991). The approaches can be roughly categorized into sequential and simultaneous approaches.

The sequential approaches to HEN synthesis are based on a decomposition of the globally complex synthesis task into a serie of simpler partial optimization problems applied sequentially. The benefit of using these approaches is the reduced complexity of the partial tasks, with the drawback that the various cost trade-offs are not properly taken into account.

The simultaneous approaches have been proposed in order to avoid this drawback. However, these approaches result generally in complex mathematical models that need simplifying assumptions (simplified superstructures, etc.) to be made in order to get practical solutions. There is often no guarantee of global optimum.

In short, the mathematical programming approaches to HEN synthesis provide "exact" solutions to approximate problems. Since the HEN synthesis in its most general form generally leads to problems of unmanageable complexity, some degree of simplification is required anyhow at some stage of the HEN synthesis process. They nevertheless offer the advantage, over competing Pinch Analysis approaches, of allowing to incorporate additional practical constraints such as forbidden, required or restricted matches, etc.

It is worth reminding that the heat recovery approach temperature (HRAT) is used as an (indirect) measure of the degree of heat recovery from a process. Temperature interval approach temperature (TIAT) is used as a parameter for partitioning into temperature intervals. Finally, the minimum approach temperature ($\Delta T_{min}$ or EMAT) specifies the minimum temperature difference between any two streams exchanging heat "through" an HEX. While in Pinch Analysis, generally no fundamental distinction is made between these three parameters (HRAT is used as $\Delta T_{min}$), this is not the case in mathematical programming, which makes a clear distinction between HRAT and TIAT=EMAT, since the optimization process can benefit from this additionnal degree of freedom (with EMAT≤HRAT).

### A.4.2.1 Sequential Synthesis Approach

The basic idea in the sequential strategy for HEN synthesis is to decompose the problem into the tasks of:

1. determining the minimum utility consumption (minimum utility costs);
2. calculating the minimum number of matches for the previously identified minimum utility target;
3. identifying the optimal HEN structure, giving the minimum investments costs, out of all possible structures embedded in a superstructure based on the results of step 2 (matches and corresponding heat rate).

This sequential optimization is done for a given heat recovery approach temperature (HRAT). Optimization with respect to this parameter is done by repeating steps 1 to 3 with as many different values of HRAT as needed.

The reason to decompose in the above three steps and to address them in this order is that steps 1 and 3 minimize the individual components of utility and investment costs, while step 2 exploits the economies of scale. The important assumption is that the energy costs are dominant, and also that the minimum number of units solution that meets the minimum utility demand is close to the minimum investment solution.

Step 1 is solved by describing the problem as a LP transshipment model (the transportation model needs a larger number of variables and constraints). Given a temperature interval approach temperature (TIAT, set equal to HRAT), the process is partitioned into temperature intervals and heat balances are written for each temperature interval, accounting for thermodynamic constraints of feasible heat transfer for cascading heat residuals.

The LP transshipment model can easily be solved by standard LP solvers and provides the required loads of hot and cold utilities, as well as the location of the pinch point(s), if any (the temperature(s) at which the heat residual is zero). The LP transshipment model supports multiple utilities.

Based on the results of step 1, step 2 consists in writing a MILP transshipment model for each subnetwork (i.e. each region between two consecutive pinch points), and solving them by branch & bound solution techniques. The MILP transshipment model explicitely includes the potential heat exchanges between all pairs of streams (except hot to cold utilities). The objective function to be minimized is the number of matches needed in each subnetwork.

The exchanged heat rate between any pair of streams is restricted by two boundary values (upper and lower). Depending on the way these bounds are set, various cases can be modelled: required, forbidden, restricted or preferred matches. The MILP transshipment model can also support the special cases of cold to cold, or hot to hot matches.

Solving the MILP transshipment models generally features multiple solutions, i.e. the same number of matches, but the matches, as well as their heat rate, may be different. Since these multiple solutions do not necessarily offer the same potential for minimizing the total investment, it has been proposed to add a (normalized) penalty factor so as to favor the solution with the highest degree of vertical heat exchange (Gundersen & Grossmann, 1990). This is done by partitioning into enthalpy intervals and calculating the maximum amount of vertical heat transfer for any match.

For step 3, a HEN superstructure is built, which embeds all the matches identified at step 2 in any type of configuration (parallel, serie, parallel-serie or vice-versa, or by-pass). The overall HEN superstructure actually consists of individual stream superstructures, which includes HEX units, mixers and splitters. The overall HEN superstructure is then formulated as an NLP optimization problem, where variables are the temperatures and flow rates of each branch of the superstructure. The total investement is to be minimized, subject to the constraints of mass balances (mixers & splitters), energy balances (mixers & exchangers), feasibility constraints for heat exchanges ($\Delta T_{min}$), and non-negativity constraints.

The NLP problem always has a feasible solution, since it has been demonstrated that it exists a one-to-one correspondence property between matches and HEX units. But even the Global Optimal Search (GOP) approach (as opposed to local NLP solvers) is not able to guarantee in practice that global solutions are found (obtaining a global solution can only be theoretically guaranteed).

In order to avoid numerical difficulties with NLP solvers, it is important to provides lower and upper bounds on all optimization variables. The tighter the bounds, the higher the probability to get good solutions. These bounds can be extracted automatically within the GAMS modeling system by performing monotonicity checks.

#### A.4.2.2 Simultaneous Synthesis Approaches

The motivation to develop simultaneous approaches, i.e. addressing the HEN synthesis as single task problem, is to be found in the intrinsic limitations of the sequential (decomposition-based) HEN synthesis approach: the trade-off between the various contributions to total costs are not properly taken into account, which can lead to suboptimal HENs.

Several simultaneous HEN synthesis approaches are described:

1. an approach which addresses the matches - HEN optimization simultaneously, while still relying on the preliminary step of targeting for minimum utility costs;
2. a general approach without any decomposition, addressing the optimization of the amount of utilities, the matches and the structure of the HEN in one step. HRAT is implicitely optimized (as opposed to approach 1, for which an external HRAT optimization loop is required);
3. a simplified simultaneous approach, postulating a simplified superstructure based upon the problem data and the assumption of stage-wise representation and isothermal stream branch mixing at the end of each stage.

In the first approach, which starts from a minimum utility cost target (for a given HRAT), the matches - HEN optimization has to simultaneously determine the matches, their heat loads and the HENs structure. The approach postulates an hyperstructure which embeds all possible matches and all possible alternative HEN structures, and formulate the problem as an MINLP based on a transshipment model and the modelization of the hyperstructure topology.

Unlike the sequential approaches, this approach does not require the decomposition into subnetworks based on the location of its pinch point(s). Hence the hyperstructure embeds the whole network, not only one subnetwork at a time. Since the one-to-one correspondence between a match and a HEX unit only holds for a subnetwork, the hyperstructure has to embed as many HEXs units as the number of pinch regions for each possible match. From the process data, all potential matches are easily identified, each individual stream-hyperstructure can be generated, with splitters and mixers so that the HEXs can be connected in whatever sequence (serie, parallel, and mixed parallel-serie).

With respect to the formulation of the constraints deriving from the transshipment model, it is worth noting that the most general case is when criss-cross heat exchanges are allowed by setting EMAT=TIAT <(<) HRAT. The degree of economically beneficial criss-crossing will automatically result from the optimization. The case EMAT=TIAT < HRAT is referred to as the pseudo-pinch case. The pseudo-pinch case is equivalent to allowing the search for cost-optimal HENs in a wider solution domain than when the strict pinch case is artificially imposed.

As already mentionned, the simultaneous matches - HEN optimization leads to an MINLP model, which is nonconvex. The solution strategy is based on the Generalized Benders Decomposition (v2-GBD). A clever decomposition into a set of y variables of the primal problem and x variables of the master problem is proposed.

Optimal HENs generated using this approach often feature parallel HEXs and non-isothermal mixing.

The second simultaneous approach to HEN optimization takes full account of trade-offs between energy costs, HEN structure, HEX costs and the economies of scale. The optimization of HRAT is implicitely included. Hence the utility loads are treated as explicit optimization variables; the pseudo-pinch case (EMAT=TIAT<<HRAT) is also considered here. Note that the decomposition into temperature intervals only depends on the supply temperature of both process and utility streams, and of course on EMAT (a practical inferior limit could be EMAT=1°C), but not on the actual amounts of each utility.

The MINLP model results from the pseudo-pinch MILP transshipment model and from the modelization of the hyperstructure topology, the same which is used for the former simultaneous match-HEN optimization.

The methodology is demonstrated on an example process; the individual stream-hyperstructure on one stream includes 5 matches (units), which implies already a quite complex hyperstructure if all possible configurations are actually to be included. However, in some cases, insight in the problem (e.g. considering the temperature level of streams) allows to eliminate a set of unlikely interconnections from the hyperstructure and hence reduce the number of variables of the model.

Due to nonconvexities, only local optimum solutions can be obtained, without guarantee that the global optimum is actually reached. The solution procedure use also the v2-GBD. Variables are partitioned into variables for the master problem (x including all continuous variables) and variable for the primal problem (y, including all integer variables representing the existence of a particular unit). HENs designed with this approach often include non-isothermal mixing, whenever this turns out to be more cost-effective, since the most general hyperstructure has been postulated.

Unlike the most general hyperstructure postulated by the second approach, the third simultaneous synthesis approach can be viewed as a simplified approach where solutions are searched for in a restricted space. In effect, this approach postulates a simplified HEN superstructure, in that the superstructure is stage-wise and assumes isothermal mixing at each stage.

The main motivation behind this simplified superstructure is to avoid any nonlinearities in the constraints of the model, hence limiting the nonlinearities in the objective function. At the same time, eliminating energy balances of mixing (due to isothermal mixing) decreases the number of constraints of the model. But since a number of potential HEN structures is not considered during the optimization (e.g. by-pass configuration, and more generally non-isothermal mixing of parallel configurations), only suboptimal (yet good) solutions can be obtained.

The number of stages to be postulated is chosed as the maximum of the number of hot streams and cold streams. Although this choice is quite arbitrary, it is based on the observation that optimal HENs do not feature a large number of HEXs. The number of stages can also be regarded as a parameter to control the structural complexity and the space of solutions, much like the concept of level proposed in the genetic algorithm approaches of Lewin *et al.* (1998) and Lewin (1998) described later.

At each stage, a stream is splitted into as many branches as the number of possible matches; hence the superstructrure is basically made of a serie of parallel HEXs units.

Unlike the other approaches, this approach does not rely on a transshipment model. Continuous variables of the model are the heat rate of HEX units (including utility units) as well as the temperature of each steam at the end of each stage. Binary variables are associated with the existence of HEX units at each stage. The set of constraints consists of:

- overall heat balance for each stream;
- heat balance for each stream at each stage;
- assignement of inlet temperatures;
- monotonicity of temperature changes at each stage;

- energy balance for utility units;
- logical constraints;
- calculation of temperature approaches.

To simplify the superstructure, utility units are often assumed to be located at the target end of process streams.

Since the objective function (the annual costs) is nonlinear and nonconvex, the solution of the resulting optimization model is local optimum.

The solutions obtained using this approach may feature more HEXs units than needed if stream splits are present. For these cases, a NLP suboptimization in which the HEN structure is fixed but the flows and temperatures are allowed to vary is proposed, which will identify the optimal split factors and the heat rate of HEXs.

### A.4.2.3 Comments

With respect to the sequential approach based on the decomposition into subnetworks at pinch(es), it is not clear whether some kind of post-optimization is performed in order to recombine the subnetworks and relax them to improve their global cost efficiency.

Cost-optimal HENs generally obtained by Mathematical Programming are structurally more complex than their Pinch Design Method (PDM) counterpart, in that the former include multiple stream splits, bypass, non-isothermal mixing, serie-parallel sequence, etc. It is not clear whether this structural complexity is a hindrance with respect to practical implementation. Quantitative comparisons with HENs generated by PDM is not provided. The sensitivity of total costs to slight modifications of the HEN structures (e.g. forcing the condition of isothermal mixing) is not analysed.

The various approaches based on Mathematical Programming are unfortunately demonstrated using almost trivial, degenerated problems, so that one cannot get an exact feeling of the actual capabilities of these methods.

Although the proposed methods are general and theoretically not limited, severe limitations should be expected for non-trivial, practical processes. For example, in the case of multiple utilities, one has to expect possible multiple pinch points, hence one has to introduce several HEXs units for one single match, and the hyperstructure might become very complex.

Would it be possible to obtain simpler (yet cost-efficient) HENs by restricting the topological complexity of hyperstructures. Could the consequence of limiting the structural complexity be evaluated *a priori* ?

# A.5 HEN Design Methods Based on Genetic Algorithms

## A.5.1 Introduction

Stochastic optimization based on Genetic Algorithms (GAs) has been succesfully applied to solve various MINLP engineering problems at LENI (Curti, 1998; Olsommer, 1998; Pelster, 1998). Therefore, GAs have been foreseen as a possible solution approach for the design of batch HENs. Several procedures based on GAs for the design of continuous HENs have recently been published (e.g. Androulakis & Venkatasubramanian, 1991; Lewin, Wang, Shalev, 1998; Lewin, 1998; Wang, Yao, Yuan, 1997). These procedures differ in their objectives, in the optimization scope assigned to GAs, in the way variables are encoded and in the GAs actually used. Thus, their review provides with a valuable source of inspiration for the further application of GAs to the design of batch HENs.

## A.5.2 Androulakis & Venkatasubramanian (1991)

GA based optimization procedures are proposed by these authors for two different kinds of problems:

1. the structural (discrete) optimization, as part of the general MINLP optimization problem, of continuous HENs;
2. the optimization of continuous non-linear functions, both unconstrained and constrained.

### *A.5.2.1 Structural Optimization of HENs*

For the design of cost optimal HENs, the search of optimum HEN structures (optimum values of discrete variables) is addressed using a GA, while the GRG2 non-linear optimizer solves the parametric optimization of the heat rate of each heat exchanger (which is a NLP problem). The GA based search procedure does not support stream splitting.

In order to be easily manipulated by the GA, an "individual" (i.e. a HEN structure) is coded as an ordered sequence of "characters". Each "character" represents a match between a hot stream and a cold stream, and has to be chosen among $n_{HPS} \times n_{CPS}$ different "characters" (where $n_{HPS}$ and $n_{CPS}$ are the numbers of hot process streams and cold process streams, respectively).

Using the proposed simple coding of HEN structures, genetic operators such as reproduction, crossover and mutation are easily related to actual changes of the HEN structure:

- by definition, reproduction lets the sequence of "characters" unchanged, i.e. the HEN structure unchanged;
- crossover actually corresponds to an exchange of subparts of the HENs structure;
- mutation, which makes a random change of a "character" in the string, physically corresponds to the change of either stream of the match which "mutates".

Hence, the actual structure of the system is used as the independant variable and not some transformation (binary coding) of it through the use of decision (0-1) variables.

Also important is the fact that a balance between random exploration and reproduction of good matches is required. A generation-dependant mutation and crossover rates is adopted (mutation rate decreases and crossover rate increases as the number of generation increases).

Good HEN designs are identified using the proposed procedure, as long as the string length (i.e. the number of HEX units of the HENs) is fixed. Obtaining not one, but a family of possible alternatives to choose from is clearly an advantage when additional performance criterias (i.e. controllability) are considered.

Optimization with variable string length failed to identify optimum HENs, because, so it is said, the dimensionality of the solution space is continuously changing.

#### *A.5.2.2*
#### *Optimization of Non-linear Continuous Functions*

The authors propose a so-called «extended genetic search» (EGS) as a mean to avoid being trapped in local optima by deterministic methods (based on gradient). The proposed EGS combines the characteristics of genetic search through recombinations and mutations of the existing solutions and the characteristics of both trajectory and clustering methods.

The direction of search is used as the independant variable. The only adjustable parameter is the step size.

Good performance on both "soft" and "hard" functions are reported, for constrained and unconstrained optimization. The EGS is particularly useful as a tool for problems where good approximate solutions are needed quickly, as it allows for a mapping of the solution space and provides deterministic solvers with good initial feasible solutions.

#### *A.5.2.3*
#### *Comments*

Several comments should be made:

- with respect to the optimization of the heat rate, given a HEN structure, no information is given on how GRG2 is actually applied and how easily optimum solutions are found;
- the required computing times to solve processes of industrial size are not given;
- the coding of the HEN structure differs from the one adopted by the authors of the following papers (refer to *Sub-section A.5.3* on page A-36, *Sub-section A.5.4* on page A-40, and *Sub-section A.5.5* on page A-44).

### A.5.3
### Lewin, Wang, Shalev (1998)

This paper actually forms Part I of a serie of two papers, Part II being that of Lewin (1998) - refer to *Sub-section A.5.4* on page A-40.

Part I addresses the synthesis of MER HENs, without resorting to stream splitting. As a design parameter, a minimum $\Delta T_{min}$ is specified for all HEXs.

The general MINLP optimization problem reduces here to a MILP (the objective function - energy recovery - being a linear function of the heat rate of each HEX, and constraints being linear in these variables).

The MILP problem is solved by a cascaded algorithm, consisting of:

- an upper level based on GA dealing with the initialization and the optimization of a population of HEN structures;
- a lower level responsible for the continuous parametric optimization of each HEN structure supplied by the upper level, based on a PL formulation and solved by a Simplex algorithm. The maximum amount of heat recovered by each HEN structure is supplied back to the upper level as a measure of its fitness, used by the GA to create the next generation of structures.

A HEN structure is described by an ordered set of integer variables, according to well defined rules. The description is organised along with the choice of key streams (either the hot or the cold streams), with their ordering (arbitrary numbering), and with the concept of HEN level. If there are more cold streams than hot streams, these should preferably be selected as key streams, in the opposite case, choose the hot streams as key streams.

The ordering of HEXs on streams is important; by convention, the corresponding structure starts from the supply side of the key streams and proceeds towards their target ends.

The concept of HEN level is a mean to organize the HEN and to control its complexity. Within a HEN level, each key stream (in their order of numbering) is allowed to be matched against a non-key stream (at the most one match per key stream at each level). Once the last key stream (the one with the highest numbering) has been considered, another sequence of possible matches is possible if the total number of levels has not yet been exceeded - otherwise the (internal) HEN structure is complete and fully defined.

The structure is represented as an (ordered) matrix of key streams versus level (incidence matrix). The matrix elements are assigned either the number of the non-key streams with which the key-streams are matched, or zero if no matches are present. Note that external heaters and coolers are automatically included at the target side of the streams and automatically warrant the heat balance of each stream.

The incidence matrix is actually represented as a one-dimensional string of integers to be manipulated (evolution by reproduction) by the GA, a task it is well suited for. The initialization of the population can be randomly made, or seeded by desired matches. After the low level LP optimization has been achieved, the returned value of the objective function (overall heat recovery for each "individual", i.e. HEN structure) is used as a fitness indicator of that individual.

The new population of structures (generation of individuals) is created by a reproduction process, in which a fraction of the individual are simply cloned (to keep the patrimony of the population), while the remaining are reproduced by crossover (exchange of parts of genetic information between the two "parents", i.e. two structures; the crossover position in the string is randomly determined). A small fraction of the new population is finally modified by random mutation (to increase diversity and explore new structures by randomly modifying the integer of one match).

For cloning as well as reproduction by crossover, the "parents" are choosen by fitness based random selection; the probability of a structure to be present in the next generation is therefore proportional to its relative fitness. At the same time, the fittest structure always survive intact from one generation to the next, so as to avoid the risk of being corrupted by genetic manipulations.

The description adopted here (based on key streams and the concept of level) warrants a constant HEN structure size whatever the manipulation of the GAs.

At the lower level, each structure out of the population provided by the upper level is translated into a LP problem, which is solved by a Simplex algorithm for maximum energy recovery. The LP is made up the objective function (the sum of the heat rate of the process-to-process HEXs) subject to the heat balance constraints for each process stream and the $\Delta T_{min}$ inequality constraints on each heat exchanger. The heat rates of the process-to-process HEXs are the independant variables of the LP problem.

The reported case studies demonstrated that good HEN designs are generated within affordable CPU times. The GENESIS 5.0 implementation of the GA has been used, with crossover rate equal to 60%, and mutation rate in the range 0.1 to 0.5%. The population size and the number of generations computed (the selected termination criteria) were taken in proportion to the chromosome length. For a process made up of 5 cold streams and 4 hot streams, the population size, the number of generation and the CPU time, respectively, have been 40 / 20 / 10 s for one level; 60 / 67 / 70 s for two levels; 80 / 100 / 240 s for three levels. The number of levels is progressively increased until a specified degree of heat recovery is reached, assuring that a minimum number of HEX units are used to achieve this target.

The GA HEN design methodology has also been applied with the process being decomposed in two regions at the pinch to compare with the conventional pinch design. MER HEN have been easily designed.

The approach is impressively simple and efficient. One major advantage over the deterministic optimization is the ability (as a standard) to supply a family of solutions which can be compared with respect to other side objectives, such as operability, controllability, etc.

### A.5.3.1 Comments

The achievable heat recovery targets are of course constrained by the specification of the $\Delta T_{min}$. The actual (MER optimized) $\Delta T_{min}$ on each HEX depends on the structure of the HEN; if the HEN structure is "compatible" with (or similar to) a pinch designed HEN, the (MER optimized) temperature driving forces of each HEX should somewhat mimic the vertical temperature driving forces available on the composites.

The structural complexity is controlled by the number of HEN levels, making the maximum number of process-to-process HEXs equal to the number of level times the number of key streams.

Nonetheless, experience and skill of the user is still required, in particular with respect of the selection of the number of levels (optimization parameter). Guidelines should be provided, based on some simple criterias: the ratio of the number of key to non-key streams, the relative contribution to total recoverable heat, the number of pinches and pseudo-pinches (hence the number of independant design regions), etc. The criterias could possibly be more complicated, as long as these could be automatically calculated.

If balanced HEN design is desired, one should first incorporate the utility streams as internal streams, then select the minimum number of level with respect to the number of pinches (utility and process pinches). If no utilities are available at the target end of process streams, the number of levels should be increased until external heaters and coolers aren't required anymore.

Choosing which streams are going to be key streams has an influence on the structure of the HEN and the number of levels, and finally on the ability to achieve a MER target within a defined number of levels. The choice can only be made globally for the whole process (unless the process is split into separate pinched problems); for one particular region, the key streams might effectively be more numerous than the non-key ones, while the opposite case might be encountered in another region.

Actually, the number of levels is an indirect mean for controlling the structural complexity; more importantly, it is the combination of the key streams and the number of levels which is the actual measure of the complexity (max. number of HEXs). If one changes the choice of key streams, one should recalculate the number of levels accordingly in order to maintain or overrun the max. number of HEXs.

Another aspect which has not been addressed yet is the ordering (numbering) of key streams, which can prevent some HEN structures to exist within a defined number of levels, i.e. whenever a match on a key stream coming later in the numbering should actually be placed before a match on a stream of lower numbering (if they should match the same non-key stream). It is not clear, in the general case, whether increasing the number of levels just by one will solve this problem.

The prohibition of stream splitting greatly simplifies the continuous parametric optimization; the influence of this assumption on the required number of HEXs to achieve a specified degree of heat recovery depends on the process under consideration; streams requiring splitting (e.g. with large heat flowrate to be matched against many other streams) shall likely require a "substitute" to splitting in the form of a sequence of serially-connected HEXs.

### A.5.4 Lewin (1998)

This paper (Part II) describes further developments of the methodology presented by Lewin, Wang, Shalev (1998) (refer to *Sub-section A.5.3* on page A-36) to address the more practice-relevant case of designing cost-optimal HENs, for which stream splitting is allowed. The methodology has been mainly modified with respect to the lower level optimization algorithm, to the description and the coding of the HEN structures, and to the NLP formulation.

The division of the problem into an upper level in which HEN structures are generated by a GA, and a lower level optimization dealing the continuous parametric optimization (and feeding back the GA with a fitness factor for each structure) still holds. The differences lie in that the objective function (the annual cost to be minimized) is non-linear in the variables of the problem (heat rates of HEX and split fractions of streams), and also in that the split fractions introduce non-linearity in the $\Delta T_{min}$ inequality constraints.

Since it is observed that cost-optimal HENs involve relatively few stream splits, and that the NLP constraints are linear in heat rates, the NLP problem is solved using a cascaded algorithm consisting of a non-linear optimization of the stream splits (while keeping constant the heat duties), followed by a pseudo-linear optimisation (modified Simplex) of the heat rates (while keeping constant the split fractions). This decomposition has been preferred to a NLP simultaneous optimization of the heat rates and the stream splits optimization based on the stochastic «Controlled Random Search» which is robust but very slow.

The simplifying assumption of isothermal mixing is not required for the splits, while the non-linearity of the objective function is actually not a problem in this case, since it is only used to evaluate the fitness of the structure at the end of the lower level optimization. Furthermore, the annual cost is actually not optimized directly, in that the objective function used in the pseudo-linear optimization of the heat rates is the heat recovered by the HEN (linear in heat rates). For algorithmic robustness, the logarithmic mean temperature difference is replaced by the Chen approximation (Chen,1987).

The description of the HEN structure is modified in two ways. Due to the now essentially parallel structures (quite similar to the spaghetti design network) of the matches within each level (because of possible splits on both the key and non-key streams, and the fact that only one match per branch is allowed), there is now no significance to the ordering of HEXs within a level.

The description of a structure is organized as level versus incidence matrix (key streams times the maximum number of branches allowed for each stream) . The number of branches of key streams is directly controlled, while this is not the case for the non-key streams, for which the random manipulations by GA could generate structures for which the maximum number of branches of non-key streams is exceeded.

Therefore, a preprocessor is introduced to perform consistency checks and correct infeasible structures. This preprocessor can also be used to define constrained matches and forbidden matches, a highly desired feature in HEN design practice. It checks also for the thermodynamically forbidden matches.

The incidence matrix (describing a HEN structure) is translated into an NLP model; independant variables are the HEX heat rates and the split fractions. The fact that equality constraints are more difficult to deal with by NLP solvers than inequality constraints, has motivated the transformation of energy balance for each stream into inequality constraints, with respect to the final temperature of the streams being "less" or equal to their target temperature (the remaining being supplied by utilities). The energy balances are independant of split fractions. The $\Delta T_{min}$ inequality constraints for each HEX are systematically calculated from the heat rates and the split fractions; this dependance on the split fractions arises from the fact that non-isothermal mixing is considered.

The NL optimization of the stream splits begins with the initial guess of equal split fractions. It has been observed that the stream split optimization is multimodal and non-convex. Within regions where the energy recovery is maximum, the total annual cost can be highly multimodal and non-convex. A two-step approach has therefore been suggested, in which initially the stream split optimization focus on the MER objective, followed by a search within this region for minimum costs. For both steps, the downhill Simplex method (with parabolic acceleration where appropriate), has been used.

The reported case studies demonstrate the efficiency of the GA-based HEN synthesis. But design parameters such as the number of levels and the number of branches for key streams and non-key streams need to be "trimmed" (starting with small values in order to limit the complexity) in order to check their influence on the cost-optimal HENs obtained. Candidate for stream splitting are identified on the basis of their relative contribution to the overall heat demand or supply, respectively. It is shown how essential matches develop and propagate through the generations, while poor matches progressively disappear. Industrial-scale problems can be solved without requiring particular initial solutions or the formulation of a superstructure.

### A.5.4.1 Comments

Apart from choosing which streams are going to be key streams, and setting the number of levels, the user has to define the maximum number of splits (branches) on key streams and on non-key streams (a stream-dependant maximum number of splits could possibly be defined). This design parameter represents an additional degree of control, but requires at the same time more skill, experience, or guidelines to be optimally used. *A priori* analysis of the problem (insight in the process) is required.

Although the GA HEN design methodology significantly outperforms other design methods on several case studies, it is not yet clear how the indirect optimization of annual costs through the maximization of recovered heat actually performs, and whether better HENs could not be found if the cost was directly optimized (or if the MER designs were slightly relaxed to optimize the annual costs). This problem might be closely related to the role played by $\Delta T_{min}$ in the optimization:

- is it possible that the cost-optimal HENs stumbles against the $\Delta T_{min}$ constraints (meaning an overall optimum exists for some smaller value of $\Delta T_{min}$) ?
- or what happens if a very low value of $\Delta T_{min}$ is specified ? Does the procedure automatically direct to the $\Delta T_{min}$ region representing the optimal trade-off between energy and capital ? Or does the methodology "simply" explore the best structures that could be designed for a preliminary identified economic optimum $\Delta T_{min}$ (e.g. by supertargeting). The fact is that for all case studies, a $\Delta T_{min}$ value has been specified as a design parameter.

It has been shown that the stream split optimization cannot focus on MER objective alone to reach cost-optimal HEN. Is the two-step approach really robust, are cost-optimal networks always to be found in the MER regions ?

As opposed to the incidence matrices for MER HENs without stream split, there are now in general several incidence matrices describing the very same HEN structure, as the ordering of matches within each level has no significance anymore. Is there a risk that HEN structures which can be described by several (many) matrices shall dominate the population ? Should the preprocessor check and convert to a standard representation after each generation ? Is there a "biais effect" due to the random modification of the structures by mean of the preprocessor ?

It would also be interesting to design cost-optimal HENs for the same problem with and without stream splits, and so evaluate the penalty resulting from assuming no stream split.

Using the preprocessor, would it be possible to apply a "probabilistic" penalty on matches of streams which are far away, or would this be better done automatically by incorporating the piping costs into the objective function ?

### A.5.5
### Wang, Yao, Yuan (1997)

Inspired by GA, a «distributed continuous-formed evolutionary algorithm» (DCEA) is proposed. In order to apply the DCEA to HEN synthesis, a general HEN superstructure has been developed. It is claimed that large-scale cost-optimal HENs can be efficiently designed.

Applied to HEN synthesis, the optimization algorithm does not involve a decomposition into an upper level dealing with structural optimization by GA, followed by a lower level where continuous parametric optimization is carried out by a relevant mathematical programming solver, as presented by Lewin, Wang, Shalev (1998), and Lewin (1998) (refer to *Sub-section A.5.3* on page A-36, and *Sub-section A.5.4* on page A-40, respectively). Instead, after postulating a general HEN superstructure for the process, the problem "reduces" to the continuous parametric optimization of the heat rate of all the possible matches contained in the superstructure. This optimization is carried out by the DCEA. This solution approach has the advantage (over other GA approaches) of not requiring any particular linear features of the problem (nature of constraints or linearity of the objective function); the only present limitation is the fact that stream splitting is not allowed.

To efficiently (i.e. quickly and with precision) optimize real variables (the heat rates), the DCEA directly manipulate real variables, without requiring them to be coded into binary strings, and decoded back to real variables (with a limited precision and a pre-specified range). The traditional genetic operators, such as crossover or mutation, involving binary strings, have been generalized to manipulate real variables. Through crossover, depending on the value of the crossover coefficient t, any "point" in the state space can be reached with a non-zero probability from any initial "point". In a similar way, a mutation coefficient s is defined and applied.

The crossover coefficient t is randomly selected in a range [0, T], where T linearly decreases as the number of generations increases. The mutation coefficient s is randomly selected in the range [-S, S], while S increases as the number of generation increases. Large T values at the beginning allows for a large initial search field. The role of mutation is to enrich the diversity to escape from possible local optima. S is progressively increased to compensate the decrease of T. In this way, a balance exists between exploitation of existing features and exploration.

Rank-based selection, or the Sqrt-rank-based selection are used to define the probability for an individual to be chosen for reproduction. In this way, the probability of "bad" individuals to survive is non-zero (their probability decreases gradually along with the increasing of generations, just like the bad acceptive probability of Simulated Annealing). This is a desired feature since the performance of an individual ("bad" or "good") should not be evaluated in a single generation; even "bad" now, it may potentially contain interesting features that require several generations to develop.

In addition, the DCEA is a subpopulation-based distributed evolutionary algorithm; the population is divided into a number of subpopulations. Each subpopulation evolves independantly for some generations, trying to locate good local optima. Then, information is exchanged between subpopulations to assemble global information. These distributed strategies include crossover between subpopulations and exchange of the best performing individuals, in a structured way.

The HEN superstructure is organized in stages. Within each stage, each stream is allowed to exchange heat with any other stream of the opposite kind. In other words, within a stage, the number of matches on any cold stream is equal to the number of hot streams. The number of stages is a design parameter selected by the user. Conventions are adopted with respect to the direction of increasing stage number, and within each stage, in which order the matches are defined. In order to obtain a completely general structure and avoid the biaising effect the arbitrary ordering of hot streams and cold streams might have on the sequence of matches in the structure, the numbering of cold and hot streams can be randomly generated.

The number of independant variables (heat rate of possible matches) to be optimized by the DCEA is equal to the number of stages times the number of hot streams times the number of cold streams. For the generation of a feasible initial population of feasible HENs, each match (in their order of definition) is assigned a heat rate randomly chosen within its feasible range.

During evolution, some individuals of the new generation may not represent feasible HENs. After reproduction, the feasibility of each HEN is checked, and excessive heat rates responsible for impossible heat transfer are systematically brought back to the maximum possible heat rate.

#### *A.5.5.1 Comments*

This optimisation approach can be considered as an intelligent, "systematic trial and error" strategy.

However, the paper does not go into some important questions, among which:

- how are the sub-populations defined and formed ?
- how are the genetic operators of DCEA actually applied to the HEN "solutions" ?
- what about the strings of integers describing the ordering of cold streams and hot streams, introduced to generate all possible superstructures ? Are all possible strings actually generated, and for each of them, is the optimization of the heat rate performed ? This seems very unlikely for the case study with 29 cold streams and 26 hot streams. Aren't many strings redundant ? Are these part of the information in the sub-populations ?
- the actual information the DCEA-based HEN design gets from a preliminary targeting or insight given by the block-based decomposition (Zhu *et al.*, 1995) is not clearly defined. Is the DCEA really able, as claimed, to start from scratch, without any information on HRAT, EMAT, etc., and automatically identify the best trade-offs, although at the expense of increased computing time ? Are near-optimal initial solutions only required to speed-up convergence ?
- are there guidelines to select the number of stages of the HEN superstructure ?

- it is not clear whether progressing systematically from the hot end of the process to the cold one for the feasibility check and possibly modifying the heat rate could biais the search or not;
- with respect to the ordering of hot streams and cold streams to be investigated, would it be possible to use physical insight to reduce the number of cases to be evaluated, e.g. by ordering them with respect to their highest temperature ?

## A.6 Conclusions

The above literature review highlights the following aspects:

- the heat integration methods suitable for batch processes do not generally consider both direct and indirect heat recovery;
- methods for the design of either direct or indirect HR schemes have been proposed, but the detailled economic optimization can't be addressed efficiently and on sound basis with the methods proposed to date. The post-optimization (PO) proposed to follow the application of the Permutation Method (PM) will unlikely provide optimal solutions;
- constraints of particular relevance in practice (e.g. contraints for the re-use of HEXs, hot process water streams) have not been (or cannot be) considered by the methodologies proposed so far;
- again, Pinch Analysis is best used for scoping and screening of major alternatives (i.e. integer decisions, e.g. with respect to the assignement of heat storage, etc.) but much less suited for detailled economic optimization (it can help in understanding why a solution is good, but cannot devise in which direction to go to improve it);
- as far as automated HEN design is concerned, it is worth noting how so many approaches (based on differents assumptions, different tools, etc.) can lead to so many different HEN structures while their economic profitability shows only small discrepancies. The costs and operational issues related to structural complexity have not been addressed so far. The ban of stream splitting can be replaced by a serie of cyclic matches, apparently without significant cost penalties. Considering the large decrease of the model complexity, the "no stream split" assumption seems justified for batch processes;

- although very general hyperstructures can be modeled, HEN design and optimization methods based on mathematical programming still bump against local optimum or complexity issues, at least for many of the processes found in practice. Either simplify the model to get the optimum solutions of approximate problems, or find approximate solution to exact problems;
- automated design and optimization methodologies for continuous HENs based on genetic algorithms (GA) have demonstrated very promising results, while the function actually assigned to the GA and the way the HEN structure is coded are quite different.

# Appendix B

# SPECIFICATIONS OF THE LENIPASS FEATURES

## B.1 Overview

As already highlighted in the intermediate report covering PinchBATCH - Phase 1 (refer to *Appendix A*), it has been recognized soon after the start of PinchBATCH that new batch features could hardly be implemented in PinchLENI, because these would require major extensions of the data structures (with unexpected side-effect in many modules) and a major reorganisation of the modules. After the leave of the major developer, the documentation and the maintenance on several operating systems were also important issues.

The availability of an EPFL-Funding for software developments in Java provided the opportunity to re-program PinchLENI in Java, which has been renamed LENIpass (LENI Process Analysis and Synthesis Software). Early development stages, exclusively concerned with the very basic tools of Pinch Analysis (composites curves, grand composites curve, and related features) are reported in *Appendix A*.

To efficiently deal with batch processes, LENIpass has been designed to include three major modules (although the boundaries between these modules appear to be less and less clearly well defined):

- LENIpfd, an essentially graphic module for process flowsheets and documentation and scheduling purposes. Equipments required to achieve a batch recipe are defined in LENIpfd; their state (i.e. the task currently being performed by the equipment as a function of time) can be represented on.the flowheet as well as on Gantt diagrams;

- LENItarget, a module providing the user with various tools and algorithms for targeting purposes, i.e. tools for the preliminary heat integration analysis ahead of any design (composites, grand composites, various supertargeting strategies, TAM model, etc.);
- LENIdesign, providing the user with facilities to design (direct) heat exchanger networks (HENs) and (indirect) heat recovery schemes including heat storage units (HSUs).

The heat integration of continuous processes could be dealt with using LENItarget and LENIdesign (two standard modules found in many process integration packages), without a major need for LENIpfd. For the analysis of batch processes, however, LENIpfd is of critical importance for process definition, scheduling, debottlenecking and more generally process understanding. Experience has schown that fixed schedule, single product batch processes are very often an over-simplified view of the reality, and even in this case process understanding requires suitable graphical representations because of the fundamental time dependance. A thorough heat integration analysis not only requires the heat recovery potential assuming a fixed schedule to be determined, but also requires rescheduling opportunities to be assessed (for energy savings or more generally for process debottlenecking, since a capacity increase is usually given a much higher priority and the associated benefits pay by the way for the related energy savings). Debottlenecking and improved heat integration opportunities can be achieved by changing the way equipments are assigned to tasks, e.g. changing from the usual in-vessel heating (and cooling, resp.) to feed preheating during charging (and cooling during discharge, resp.); Gantt diagrams are required to this end. The need for a LENIpfd module arises from the fact that batch processes feature very close links between the recipe and tasks definitions, the assignement of equipments to tasks, the scheduling and the resulting heat recovery potential and related costs.

In order for LENIpass to meet the expectations of end-users (engineers from consulting companies, from industry, etc.), it has been suggested that they should participate in the definition of these features. A first attempt has been made in the frame of the Swiss National Team on Process Integration (CH NT-PI). It failed because of a lack of experience in or even awareness of the existing tools and methods for heat integration of batch processes, and most generally a lack of time. Establishing a list of specifications and their interactions requires a significant amount of time (numerous one-to-one, in-depth discussions), which seems impossible to find for most of the CH NT-PI members.

The rate of implementation of LENIpass is significantly lower than expected, for the following reasons:

- in order for the software to be suitable in industrial practice, the general organization (data management, user interface, etc.) had to be given due consideration. To this respect, the existing PinchLENI did not provide help. The amount of time needed to this end has been largely underestimated, as a result from the insufficiently experienced and sub-critical development team;
- Java underwent several major revisions during the development of LENIpass. This lack of stability and the need to benefit from new features required significant re-programming of the code. Java has developed from a simple object-oriented programming language into a very complete (and complex) environment, difficult to manage by a single programmer;
- the early leave of the main programmer has stoped the development process. In addition, it turned out that experienced java programmer are very difficult to find, since the demand form the private industry is high at very attractive conditions;
- the almost simultaneous development of methods and their implementation in an end-user oriented software is a objective difficult to meet.

Hence, the state of implementation of LENIpass is still quite low:

- LENIpfd implements the basic features of a flowsheeting tools, while all other features (e.g. scheduling) have only been specified in details but not yet implemented
- LENItarget implements the calculation and the representation of composites curves and grand composite curve, including some usefull facilities. A stream editor is in development, while the targeting features have only been specified;
- for LENIdesign, only preliminary draft specifications are available at this stage.

Although the actual implementation rate is still below expectations, a significant potential has been developed under the form of a cluster of specifications that remains to be converted into a practical software.

The following sections describe in more details the state of LENIpass and its 3 main modules.

Note that a simple software tool for the batch industry has recently been developed by Interduct (Delft University Clean Technology Institute) (Stikkelman, 1999). The software is intended for a quick assessment of the energy, water and waste saving potentials, to be obtained typically within a half day, so as to decide whether a further detailled analysis is justified or not. To this end, the software implements very simple models and "rule of thumb" calculations (not based on any energy or water pinch calculations, but rather identifying some individual significant opportunities).

## B.2 PinchLENI

The features implemented in the PinchLENI software are described in the intermediate report PinchBATCH - Phase 1 (refer to *Appendix A*). No additional feature has been implemented during PinchBATCH - Phase 2.

## B.3 LENIpass

### B.3.1 General Organization, Graphical User Interface

In order for a software package to be suitable for industrial practice, the following characteristics were identified to be of particular relevance:

- an almost self-explained organization (a clear underlying "philosophy"), so that the user feels confident and intuitively understands how to use it;
- a sensible way of organizing the numerous files generated along the course of a project (case study) into a hierarchy of files, and a clear strategy to save, update and interchange data between the modules. Well-defined rules for updating related windows are also needed (e.g. changing the pinch of composite curves and automatically reporting this change on the grand composite, if represented);
- a uniform and standard graphical user interface (uniform meaning that whatever the module or the situation, similar actions are associated the same meaning, while standard means the interface has common "look and

feel" and uses actions that are usual to other software tools). A need to avoid the multiplicity of commands to perform the same action;

- a contextual help providing suggestions and guidance, since the unregular user of Pinch Analysis is often confused by the great variety of tools and methods, not knowing which ones are relevant to his problem, and as important, in which order (Pinch Analysis is much more a toolbox than a linear, regular strategy to reach a single goal);
- the opportunity to select the actual units and formats of both input and output data among a set of available units and formats (while internal units are invariable);
- standard facilities for graphs to represent any single (or couple of) parameter as function of any other parameters, allowing for various axis scales, and providing cursors measurement.

With respect to maintenance and further development, encapsulation provided by object oriented programming is helpful. In addition, the organization into beans (a Java concept of self-contained modules) is very powerful in customizing the modules, the content of windows, etc., at the expense of spending more time during the conceptual phase for the definition of the beans, the way they communicate, etc.

To meet the above need, specifications have been produced so far for:

- the GUI and the organization of the working space of LENIpass into sheets (somewhat similar to Excel), on which different windows can be represented;
- the basic principles of the contextual help. Analysis options available at any time depend on the defined data at this time;
- selectable units and numerical data formats;
- the calculation and representation of graphs with related options;
- the data editors and data lists,which are to be used througout the modules;
- the organization and part of the management of project data; the organization of data into a hierarchy of files and the obligation to modify data at its highest level of definition (reflecting the propagation of changes. i.e. dependancy of files) should prevent data inconsistency to develop through the course of the project, since it forces the user to make sure the considered changes are actually feasible, given the other process data. This means that if the user is only interested in representing

composites curves of a set of streams, he/she will not spend time to first define a list of equipments, assigne tasks, etc. (in this case, these informations would be arbitrary anyhow) but rather directly define a stream table. But if he/she intends to make changes to an existing process which has been defined by equipments, tasks, schedule, etc., modifications should be made at the appropriate hierarchy level so that changes will propagate downwards.
However, Process (Heat) Integration using Pinch Analysis generally requires several alternatives to be assessed; therefore the user has to be provided with shortcuts to quickly assess any potential solution - without spending to much time if the solution fails. LENIpass shall be provided with such shortcuts: the user makes a copy of the original stream table, which he can directly edit. Once major alternatives have been assessed and decisions made, modifications can be made to the original, unaltered table via the higher data levels;

- the objects (data units) at the root of LENIpass: fluid, equipment, stream, schedule, etc.
- systematic rules for consistency check and data update; conventions for representing editable and non-editable data, check box to highlight which data is specified or calculated, etc.

The suggested hierarchy of folders and files mimics the structuration of a production site in plant (including plant-wide utilities and toal site integration issues), building (including related equipment lists, definition of process recipes by tasks and required equipments), macro-scheduling (various production planning scenarios), alternate time period analysis. etc. process, etc.

## B.3.2
## LENIpfd Module

LENIpfd is basically a graphic module for process flowsheet, documentation and scheduling purposes. The equipments required to achieve a batch recipe are best defined in LENIpfd; their state (i.e. the task currently being performed by the equipment as a function of time) can be represented on the flowheet as well as on Gantt Diagrams. The need for this module in the context of batch processes has been explained in *Section B.1.*

The basic graphic facilities needed to draw process flow diagrams (PFDs) and for the addition of comments for documentation purposes is available as a separate module (not yet included in LENIpass).The introduction of facilities to export PFDs (i.e. copy/paste) and changes to support a "clean graphic mode" (provided by Java 2D) is under way. Specifications for over 200 graphical equipment symbols have been produced (mainly DIN and BS symbols, with some additional branch-specific symbols) and about 100 have already been implemented, while a simple description language allows any user to define additional symbols.

Other LENIpfd related activities (stream extraction from PFDs, scheduling, macro-scheduling, etc.) have been specified to a large extend but are not yet implemented. The specifications are summarized below in their normal chronological order. Note that drawing a PFD is not necessarily the first activity to start with, and a quick alternative to define the process is also provided.

1. First, a list of equipments (ressources) available in a plant is created. The list includes, for each equipment, its type (model), an identification number, an its mode of operation - batch, semi-continuous, continuous - (read-only information, derived from equipment model). Additional data (such as equipement capacity, material, etc.) can be defined using an equipment editor.
2. Once the list of available equipments has been specified, the list of equipments to be used for each process (recipe) to be achieved in the plant has to be defined. This is done by specifying a process (recipe) name and specifiying (or modifying) the equipments actually used, i.e. the user ticks off the corresponding equipments. Pieces of equipment working out-of-phase (to avoid a time bottleneck) or in-phase (to remove a capacity bottleneck) are specified by groups.
3. After the definition of the subsets of equipments to be used for each recipe has been completed, the way the equipments shall be assigned to perform recipe tasks (and related thermal streams) has to be specified. This is done by specifying the task name, the related thermal stream(s) (if any), the start and stop times (relative to the origin t=0 time of the batch), and the assigned equipment(s) (several equipments are specified for semi-continuous / continuous tasks: from ... to ... via ...). Master/slave groups of streams are also specified. This defines all schedule related information of each of the process (recipe). Overlaping tasks (e.g. vessel heating while still loading feed) are allowed. At this stage, (thermal) process streams are still only defined by a name, the related equipment(s) (location), the start

/ stop times (relative to the arbitrary start of the recipe), and master/slave information (if any).

4. Next, for each process (recipe), additional stream related data have to be specified. The list of data, their default (internal) unit, type, and description, is summarized in *Table B-1*. Some parameters might be

| Data | Units | Type | Description and comments |
|---|---|---|---|
| Process | [-] | string in a list | Name of the process / product the stream belongs to (only meaningfull when a particular time span has been selected for heat integration analysis; mainly needed for time slice representation of streams) |
| Batch Number | [-] | integer | The batch number stream belongs to (only meaningfull when a particular time span has been selected for heat integration analysis; mainly needed for time slice representation of streams) |
| Stream Name | [-] | string | Name of the stream (e.g. summarizing the processsing step and the product being processed - up to the user). Comes from "Tasks & Streams" and cannot be edited later. |
| Material | [-] | string | Specification of the material to find physical properties in a database - to be implemented later (Model stream). |
| Thermo-physical Compatibility Group | [-] | integer | Number defining a group of streams with compatible thermo-physical properties (with respect to the re-use of heat exchangers). Default is "none" (no integer value specified, i.e. not compatible with any other streams. Is only specified once the time span for heat integration analysis has been choosen. |

**Table B-1** Parameter list of a batch process stream.

| Data | Units | Type | Description and comments |
|---|---|---|---|
| Chemical Compatibility Group | [-] | integer | Number defining a group of streams with compatible chemical properties (full or conditional) with respect to the re-use of heat exchangers.I. If conditionnally compatible, cleaning costs should be specified (remains to be further specified). Default is "none" (no integer value specified, i.e. not compatible with any other streams. Is only specified once the time span for heat integration analysis has been choosen. |
| Segment Nr. | [-] | integer | Numbering of the segment (for streams made of several segments, either for phase change or for significant changes ofCp). |
| Non-Flowing | [-] | boolean | Stream is either flowing or specified as non-flowing. Default=Not "Non-Flowing" . i.e. flowing ! |
| Time Segm. Nr. | [-] | integer | If stream is non-flowing (i.e. in vessel heating or cooling), might be decomposed into one or several time segments. |
| Latent | [-] | boolean | Stream is either of sensible heat type or latent heat type. Default=Not "Latent", i.e. "Sensible" |
| $t_{start}$ | [min] | real | Time when the stream starts to exist. Comes from "Tasks & Streams" and cannot be edited. |
| $t_{stop}$ | [min] | real | Time when the stream ceases to exist. Comes from "Tasks & Streams" and cannot be edited. |
| Duration | [min] | real | Calculated from $t_{start}$ and $t_{stop}$ |
| $T_S$ | [°C] | real | Supply temperature. |
| $T_T$ | [°C] | real | Target temperature. |
| $x_S$ | [-] | real | Supply vapor quality (or fraction). |
| $x_p$ | [-] | real | Target vapor quality (or fraction). |
| $M$ | [kg] | real | Mass of material of the stream to be processed - remember the effect of thermal inertia of equipment on batch streams -> account for increase of mass. |

**Table B-1** Parameter list of a batch process stream.

| Data | Units | Type | Description and comments |
|---|---|---|---|
| $\dot{M}$ | [kg/s] | real | Mass flowrate of material to be processed. Calculated from $M$. |
| $c_p$ | [kJ/kg°C] | real | Specific heat (for sensible heat stream). |
| $q_{lat}$ | [kJ/kg] | real | Latent heat (for latent heat stream). |
| $P$ | [bar] | real | Operating pressure (not compulsory if not a "model stream"). |
| $\Delta H$ | [kWh] | real | Stream heat (>0 for hot stream, <0 for cold stream). Calculated. |
| $\Delta \dot{H}$ | [kW] | real | Stream heat rate (>0 for hot stream, <0 for cold stream). Calculated. |
| Hot Cold | [-] | boolean | Stream either cold or hot. Automatically set according to $\Delta H$. |
| $h$ | [W/m$^2$°C] | real | Stream-wise heat transfer film coefficient (not compulsory, uses the default film coefficient if not specified). |
| Location | [-] | a sub-set of equipments | Describe in which batch equipment unit (non-flowing stream) or from which equipment to which equipment (either batch or semi-continuous - flowing stream) the stream is moved. Comes from "Tasks & Streams". |
| Add one unit | [-] | boolean | If a stream has several segments, specify whether the segments shall require one more heat exchanger unit or not (might be segmented or, less often, time segmented). Default=Not "Add one unit". |
| Optional | [-] | boolean | Optional stream (or segment). For soft streams or streams that are recovery opportunities but are not part of the process streams. Default=Not "Optional". |
| M/S group | [-] | string (?integer) | Describes the cause-to-effect relationship between streams (in particular those arising from the same task), for rescheduling purposes. Either M i for master i, or S i for slave to master i, or " " (i.e. left blank) Comes from "Tasks & Streams". |

**Table B-1** Parameter list of a batch process stream.

| Data | Units | Type | Description and comments |
|---|---|---|---|
| Rescheduling | [-] | boolean | Streams that may be rescheduled (either systematically, or from batch to batch, e.g. for synchronisation with other streams). Default=Not "Rescheduling". |
| Advance | [min] | integer | If the stream may be rescheduled, specify the max. amount of minutes that the stream may be advanced(limited by stability time reason). Default=0 [min]. |
| Delay | [min] | integer | If the stream may be rescheduled, specify the max. amount of minutes that the stream may be delayed). Default=0 [min]. |
| Modify rate | [-] | boolean | If the stream may be rescheduled, this flag indicates if the flowrate of the stream may be modified. Default=Not "Modify rate". |
| No integration (external utility !) | [-] | boolean | Stream which needs 100% an external utility (in particular for temperature level reason or controllability reason -> does not require a time slice for itself in advanced MBC targeting, and is totally isolated from the heat integration problem. Default="no". |
| No direct integration (utility !) | [-] | boolean | Specify if the stream cannot be integrated by process to process heat exchange, but only with an intermediaite utility - (e.g. critical streams such as reaction, distillation, etc. ). Default="no". |
| Hot water ("Storable" process stream) | [-] | boolean | Describe a process stream which may be easily stored, i.e. prepared at any convenient time and not required to be prepared "on-line", and may additionaly serve as heat storage media. Does not require a time slice for itself in advanced MBC targeting(and may serve as heat storage media at the same time). Default="no". |

**Table B-1** Parameter list of a batch process stream.

specified in more suitable ways. This holds for rescheduling opportunities, which are difficult to specify since they are obviously related to other streams. Note that a need for segmentation of time segmented streams (non-flowing) does not exist.

5. Once the specification of the detailed stream data has been completed, it remains to be specified in which sequence the processes (product recipes) are going to be produced, e.g. whether single batch, overlaping batches, repeated sequences of different processes, etc. This activity is related to short term production planning; in the context of LENIpass, this is called macro-scheduling. Macro-scheduling is defined by a list of processes and their (absolute) starting time. Possible infeasible time specifications due to bottlenecks are automatically checked for during macro-scheduling definition, and corrected (equipment working out-of-phase are automatically assigned in turn and bottleneck problems checked for correspondingly). Any sequence of processes is easily defined.

6. In a related window, the specified macro-scheduling, the process streams and the so-defined time slices can be represented as Gantt charts. Three types of Gantt diagrams are proposed: • an overview one, representing the occupancy (processing) state of an equipment unit by a single line (bar), without any details on individual tasks performed by the equipment or related streams, except the macro-schedule time data, and time cursors; • a group of two (time-related) detailed charts, one representing the various tasks assigned to each equipment, including charge, transfer, and discharge, and a graph representing exclusively the process streams, including time data and the decomposition into time slices. Based on any of these three graphs, periods of analysis (batch cycle time, startup or shutdown phase, etc.) can be defined and associated streams saved as particular "process" stream table. To avoid incoherence in the data files, these "process" stream tables can later be viewed but cannot be modified (refer rules defined in *Sub-section B.3.1* for modifying the stream parameters). Each Gantt diagram may be selected to display all equipments (or streams, resp.) as default, or focus on a subset of user-selected equipements (or streams, resp.).

Macro-scheduling and representations by Gantt diagrams are the last activities for the detailed definition of the "process" stream table, before heat integration analysis and targeting can take place. With respect to the functions actually assigned to LENIpfd, it should rather be renamed to LENIprodef, «prodef» standing for Problem Definition ! Utility definition (after analysis of the grand composite in LENItarget) is also a function to be carried out in LENIprodef. It should be recognized, however, that a distinction and classification of actions into problem definition, targeting or design is not always obvious and somehow arbitrary.

The number of equipments, and the degree of refinement for the definition of tasks and sub-tasks is up to the user, depending on the modelization level he/she is interested in, or rather on the objective of the analysis. This can also range from simple single-product batch plant models (requiring only about 5 to 15 minutes to be defined), to complicated, multi-product producion planning, with fine time definition.

The basic specifications for the extraction of process streams from the PFD have also been established. Equipments used to draw a PFD are not simply a graphic symbol, but are asssociated additional properties helping in the definition of process streams.

### B.3.3 LENItarget Module

The LENItarget module shall includes tools and methods (algorithms, graphs) which are used for the preliminary assessment of performance indexes at the conceptual design stage: energy, area, number of units, costs, etc. The conceptual design stage also aims at selecting utilities, opportunities for rescheduling, etc. The multiplicity of problem categories (continuous / batch, direct / indirect / mixed heat integration mode, with / without "soft" streams, grassroot / retrofit design, single / multiple utilities), targeting methods (from simple energy targeting to advanced total costs targets (both for continuous and batch processes) requires special care; a unified framework is needed, which should also allow for additional methods and tools to be easily introduced.

Utilities as well as HEXs and HSUs are equipments, with a particular focus on costs parameters. Therefore they should rather be defined in LENIpfd, like any other equipment; but their close link to targeting makes them better described in LENItarget.

The user should be provided with a list of utility models (each including economical parameters), from which he/she can choose (and modify parameters if needed) to define the actual utilities available on-site. Minimum and maximum instantaneous heat rate, possible ratio between utilities (e.g. evaporator and condenser of a heat pump, etc) could also be specified. Selection of a utility to be applied to a process requires a single utility model name to be specified.

Like utility models, a list of heat exchanger models should be available, each with its particular (adjustable) cost function. In addition, a default general model (an average, general purpose HEX) for simple preliminary targeting purposes should be included. These models shall be used for match-wise HEX specification for advanced, realistic supertargeting: in a cold stream versus hot stream matrix, each feasible match is assigned a HEX type (unless the default HEX is suitable). This is a problem specification and is more related to LENIpfd.

A general purpose and specific HSU models are also to be defined.

For batch as well as for continuous processes, various types of targeting methods (algorithms) are required, depending on the analysis stage and related data quality, the pursued objectives, e.g. comparison or sensitivity analysis purposes. The comparison of the TAM energy targets with the TSM energy targets at the same $\Delta T_{min}$ is a commonly used indicator to identify a signicant need for heat storage or to reschedule process streams. But these targeting modes are by far not suitable for total annual costs (TAC) supertargeting of batch processes.

First, targeting modes are classified according to the their relevance for continuous, semi-continuous or batch processes (i.e. the available targeting mode at any given time depends on the type of the process under consideration).

Within each class, it is proposed that "targeting modes" be defined by the user (a default, standard targeting mode shall always be provided for ease of use). A targeting mode defines which data are going to be calculated, how these are going to be calculated (i.e. the targeting algorithm), the objective function (economic model, e.g. whether TAC or NPC) and the costs contributions to include in it (e.g. including or excluding piping/valving costs in case of HEX re-use, etc.). The default graph representing the results is also defined, among the data which are calculated by the targeting model (while any other calculated data may alternatively be selected).

The window for the definition of targeting modes include all possible options, while active options depend on existing data). Once defined, a targeting model may be save and applied as many times as desired.

Before applying a targeting mode, a process stream table, a utility stream table, a HEX specification matrix (if required) should be selected (be active).

In addition to the utilities available on site, the utility stream table also includes two default utilities, which are automatically adjusted to suit at the end of process composites (just like PinchLENI for MacIntosh presently does). This avoids current problems (e.g. with PinchLENI PC) when the user has to specify utilities while he still has no idea of how the composites curves look like, or when he would simply make a very preliminary analysis. In such a case, the user shall explicitely select the default utilities. At least one hot and one cold utility have to be specified as variable, while specifying fixed heat rate of other utilities is always possible. In addition, the heat rate of the different utilities can be defined from the grand composite, e.g. so as to feature a well defined pinch ratio compared to the process pinch (e.g. same as process pinch (1/1), or a higher value).

Depending on the selected targeting mode, additional info may be required (e.g. the number of storage for indirect heat recovery, or whether soft streams are included of excluded, etc.). Before running the targeting mode, the range of targeting has to be specified (this can also be limited to a point). Again, a default range (full) is always possible for ease of use, but advanced specification is also required, which include: the range variable (e.g. the process pinch, the high utility, the low utility, the heat recovery), the range of variation and the minimum number of steps (in addition, the specified targeting functions are calculated at all intermediate singular points of the composites curves). Results from a targeting can be saved - this is particularly important for advanced targeting modes since they may be time consuming to calculate.

Targeting calculations and the representation of composite curves (composites, balanced composites, process or utility grand composite, etc.) are not related as is the case for PinchLENI.

Batch processes require an even wider variety of targeting routes and related tools (e.g. TAM / TSM models, MBC supertargeting for direct heat integration, definition of the minimum number of HSUs as a function of heat recovery, etc.). It isn't yet clear how these can be organized in a coherent way for the user not to get lost and data management to be feasible.

### B.3.4 LENIdesign Module

The LENIdesign module is the least specified module at present. As for targeting, the various cases to consider (e.g. continuous / batch, direct /

indirect heat recovery) and various design methods (e.g. manual, automated simplified heuristic, automated using GA) should be organized in a coherent and self-explained way. Additional design tools may be needed (e.g. driving force plot, remaining problem analysis, a match editor).

Nevertherless, present limitations of PinchLENI (e.g. the lack of mixers, by-pass and valves, misleading representation of streams which do not cross the pinch, the opportunity to impose the area of a match, not only its heat rate or temperature, the misleading indication of a mean $c_p$ for multi-segment streams, difficult multiple pinch design, cross-pinch HEXs are not allowed - but needed in MBC/batch HEX design, the impossibility to delete HEXs while other HEXs exist "downwards away from the pinch", etc.) have been identified and solutions proposed. Several of the above limitations are critical for batch HENs.

The HEX model in PinchLENI is very simple and allows a straighforward calculation of remaining HEX variables (linear relation between heat rate and temperatures). If a HEX is moved, PinchLENI assumes that the heat rate is conserved (while actually the area is conserved !); this assumption simplifies the calculation of the new temperature distribution through the HEN, but is not suitable for batch HENs, in which HEXs are often re-used across time slices. Therefore, a general HEX model has been developed and implemented as a Java Bean; the model can solve remaining HEX design and operating variables from any consistent set of specified variables. This HEX solver shall be present "behind" every HEX placed on the grid diagram.

With the need for not only HEXs, but also (external) coolers and heaters, splitters, mixers, bypass and valves, the HEN design obviously evolves towards a specialized drawing software, and simple rules are proposed for placing the above objects from a "graphic palette" on the grid diagram. Each of these equipments are associated with design and operational data; default cases (e.g. HEX specified by heat rate, isothermal mixing) may readily specified on the grid diagram for ease of user, while advanced specifications (e.g. HEX re-used with constant area, non-isothermal mixing) required the equipment editor window to be opened (e.g. by double-ckick on the equipment symbol).

The pinch design rules (no heat transfer accross the pinch, respect $\Delta T \geq \Delta T_{min}$ for any HEX) as applied by PinchLENI are certainly valuable guidelines for the designer, since he cannot overlook these rules by mistake. But in several cases, these rules are rather "too hard", and in the case of batch HENs), have to be passed over in several cases to efficiently re-use existing HEX area. It is therefore proposed that the design rules are applied by default (as standard), but each time a warning is issued, the user is given the opportunity to skip the message and overlook the rules.

The design of indirect heat recovery (manual or automated) requires in addition heat storage units and storage streams to be generated / placed on the grid diagram. In this context, it should be possible to merge (in part) hot process water streams with different target temperatures, to represent what is actually done in practice and to correctly model the actually required number of HEXs. From the viewpoint of the quality of the provided results, the heuristic, Pinch Analysis based method for the design of indirect HR schemes proposed in *Chapter 2* is halfway between targeting and design. But it is easier to analyse with the grid diagram; the graphical tool to analyse rescheduling opportunities to decrease the capacity of storage sub-systems is to be implemented in this context, e.g. under a Rescheduling menu.

In summary, although several HEN design issues have been analysed and solutions proposed, the specifications are by far not complete, and significant work remains to be done if the user has to be provided with efficient interactive and/or automated HEN design tools. Note that the retrofit design remains a totally unaddressed issue !