

Forty years of Heat Integration: Pinch Analysis (PA) and Mathematical Programming (MP)

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Process Integration (PI) supporting Process Design, Integration, and Optimisation has been around from the early 1970s. PI was developed originally from Heat Integration, which remains the cornerstone for PI continuous advance. It has been closely related to the development of Chemical, Mechanical and Power Engineering supported by the extended implementation of mathematical modelling, simulation and optimisation, and by the application of information technology. Its development has accelerated over the years as its methodology has been able to provide answers and support for important issues regarding economic development — better utilisation and savings regarding energy, water, and other resources. This contribution is targeting towards providing at least a short overview of its historical development, achievements, and future challenges.

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Introduction

Reducing and economising of resource consumption can be achieved by increasing the internal recycling and re-use of energy and material streams. Projects for improving process resource efficiencies have proven to be beneficial and also potentially improve the public's perceptions of companies. Motivating, launching, and carrying out such projects, however, involves proper optimisation, based on adequate process models. Several methodologies began to emerge during the 1970s as a response to those industrial and societal challenges connected with the oil crises and a need to use this resources more economically. One of them was 'Process System

Engineering (PSE)' [1•] and later extended again by Sargent [2••]. Contributing methodology that received world prominence was 'Process Integration (PI)' — at that time more precisely 'Heat Integration (HI)' based on PA (Pinch Analysis) [3••]. HI was formulated within the book presented by Linnhoff *et al.* [4••] that has been reprinted several times — last updated edition, Linnhoff *et al.* [5•]. Its development was further contributed to by a number of works from UMIST, Manchester, UK and other research groups in the US, Europe, and more recently by a strong contribution from Asia.

What is Heat Integration (HI)?

PI, which covers a wider scope of tasks, is a family of methodologies for combining several parts of processes or whole processes for reducing the consumption of resources or harmful emissions into the environment. It started mainly as PA based HI stimulated by the energy crises of the 1970s. HI has been extensively used in the processing (as chemical, petrochemical, pulp and paper, food and drinks, steel making) and power generating industries over the last 40 years. It examines the potential for improving and optimising the heat exchange between heat sources and sinks in order to reduce the amount of external heating and cooling, together with the related cost and emissions. It provides systematic design procedures for energy recovery networks.

HI has several definitions, almost invariably referring to the thermal combinations of steady-state process streams or batch operations for achieving heat recovery via heat-exchange. More broadly, the definition of PI, as adopted by the International Energy Agency [6•] reads as:

'Systematic and General Methods for Designing Integrated Production Systems ranging from Individual Processes to Total Sites, with special emphasis on the Efficient Use of Energy and reducing Environmental Effects.'

A general PI definition that can also be applied to HI, was presented by El-Halwagi [7•] by defining:

PI as a holistic approach to process design and operation that emphasises the unity of the process.

Reducing an external heating utility is usually accompanied by an equivalent reduction in the cooling utility demand [3••]. This also tends to reduce the CO₂ emissions from the corresponding sites [88••].

Besides HI, Water (Mass) Integration was also developed for reducing waste water effluents based on PA that can also lead to reduced fresh water intake [8^{••}]. The corresponding Mass Pinch, developed by El-Halwagi and Manousiouthakis [9], which has a number of industrial applications whenever process streams are exchanging mass within a number of mass transfer units such as absorbers, extractors, etc. El-Halwagi [7[•]] and later by [10^{••}] also published books covering HI, however his main domain has been Mass Integration. More information about other HI related developments can be found elsewhere — Klemeš [11^{••}] and also Klemeš and Varbanov [12].

The history and development of HI

HI has never lost the interest of researchers during the last 40 years and has even been flourishing recently. HI has proved itself to be a considerable potential for reducing the overall energy demand and emissions across a site, leading to a more effective and efficient site utility system. One of the first works was Hohmann [13^{••}] in his PhD thesis at the University of Southern California, USA. His work introduced thermodynamics-based reasoning for evaluating the minimum energy requirements of a Heat Exchanger Network (HEN) synthesis problem. Various approaches dealing with the optimum HEN synthesis have since been published. Some of them became very popular, such as [14]. The comprehensive overview of HEN synthesis presented by Gundersen and Naess [15[•]] and the overview of process synthesis presented earlier by Nishida *et al.* [16[•]] provided considerable impetus for further research and development within this field — as can be witnessed in the more recent overview by Furman and Sahinidis [17].

The concept of HI based on Recovery Pinch was built upon in Hohmann's PhD thesis [13^{••}] by two research groups: firstly, the two part paper of Linnhoff and Flower [3^{••}] and Flower and Linnhoff [18^{••}], followed up by the Linnhoff PhD thesis [19^{••}] and secondly, by the group around Umeda *et al.* [20[•]]. Hohmann [13^{••}] is considered to be the first to provide a systematic way of obtaining energy targets by using his Feasibility Table. In his PhD, some basic principles were included. However, with the exception of a conference presentation [21], the results were not extensively published. A lesser known part leading to the Problem Table Algorithm (PTA) was published at that time by MSc student Bodo Linnhoff at ETH Zurich [22[•]]. During those pre-information technology times, interactions amongst researchers were slower and more difficult. Discovering what other researchers were working on was only possible after acquiring printed publications. During the remaining part of the 1970s, it was again (at that time a PhD student) Bodo Linnhoff at the University of Leeds who perused and realised the potential of HI. The beginning was difficult as his first paper [3^{••}], which later became very

highly cited (258 citations in SCOPUS by 04/09/2013), was nearly rejected by a leading journal of that time. Bodo's strong will and persistence succeeded in getting the idea published and off the ground. After the first paper's initial difficult birth, others — Flower and Linnhoff [18^{••}] and Flower and Linnhoff [23] — followed smoothly.

The other group that produced interesting contributions was from Japan — at the Chiyoda Chemical Engineering & Construction Co., Ltd. Tsurumi, Yokohama. They published a series of publications on HEN synthesis — Umeda *et al.* [20[•]], Umeda *et al.* [24[•]], optimum water re-allocation in a refinery — Takama *et al.* [25[•]], and applications of the Temperature-Enthalpy (T-Q) diagram for heat-integrated system synthesis — Itoh *et al.* [26[•]].

The publication of the first 'red book' by Linnhoff *et al.* [4^{••}] played a key role in the dissemination of HI. Later this book received a new Foreword [5[•]] and content update. This 'red book' provided an insight into the more common process network design problems, including HEN synthesis, heat recovery targeting, and selecting multiple utilities. As a spin-off the Leeds University research group were published some works originating in Central Europe. Firstly, Klemeš and Ptáčník [27] presented an attempt to computerise HI [28], followed by HEN synthesis development and on mathematical methods for HENs [29]. The full scale development and application of these methodologies were pioneered by the Department of Process Integration, UMIST (now the Centre for Process Integration, CEAS, at The University of Manchester) in the 1980s and 1990s. Amongst other earlier key publications was [30^{••}] with presently more than 433 citations in SCOPUS, followed by a number of works dealing with extensions, see for example the summary by Smith *et al.* [31], first updated Russian version [32[•]] and further updated version Smith [33^{••}]. A specific food industry overview of HI was presented by Klemeš and Perry [34] in a book edited by Klemeš *et al.* [35[•]] and more recently by Klemeš *et al.* [36^{••}]. Singhvi and Shenoy [37], apply PA to a supply chain problem, where the quality is time while the quantity is material load and Lam *et al.* [38] modified the Composite Curve to relate regional land use with resource planning with 'quality' being cumulative area and 'quantity' being cumulative energy balance. Tan and Foo [39[•]] successfully applied the PA approach firstly developed from HI to carbon-constrained energy sector planning. Later Foo *et al.* [40] applied the cascade analysis technique to carbon and footprint-constrained energy planning.

Mathematical Programming concept of Process Integration

In principle, PI methods rely on three different concepts — on heuristics (engineering experience and intuition), on thermodynamics (physical insights as PA-based

HI — by [30^{••}]), and Mathematical Programming (MP), for example [41[•]]. As those relying on heuristics became more and more redundant, PI thus converged into two complementary schools of concepts, where the main contribution of thermodynamics (PA) one is in generating ideas based on engineering creativity whilst the main role of MP is to upgrade those ideas (and also generate new ones) by formulating them in mathematical forms in order to obtain optimal and feasible solutions of complex problems. Appropriate trade-offs between raw materials, operating and investment costs, and product income can be established by applying MP over overall systems simultaneously, thus obtaining truly integrated solutions. As can be seen, MP, which is related to HI, is based on Process Synthesis and Process Optimisation. It deals mainly with the HI, synthesis or retrofit of HEN, and simultaneous HI and optimisation or synthesis of process schemes and process subsystems. It is interesting to note that the ultimate effect of the simultaneous approach is not only the expected reduction in utility consumption but also the reduction in raw material intake [42^{••}]. As an important aspect of applying MP, it can be considered that new insights can be revealed by examining optimal solutions.

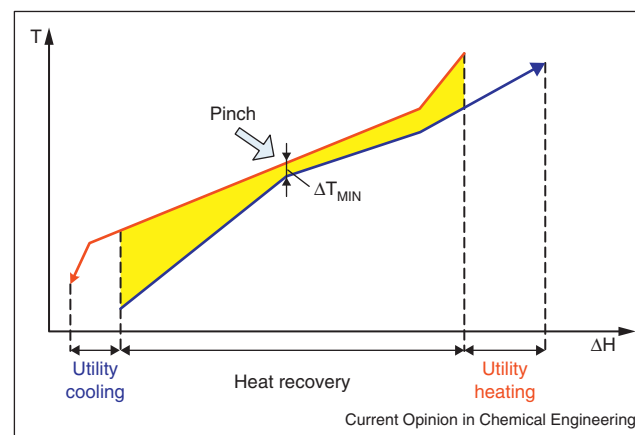
Over the past two decades several excellent review papers and books have been published within the area of the MP approach to PI. The book by Biegler *et al.* [43^{••}] deals with algorithmic methods and fundamental design concepts for PI. Another two books, one by Smith [33^{••}] and another by Klemeš *et al.* [36^{••}], also provide some basic material on the MP approach to PI, amongst a wealth of knowledge about PI. A review of the algorithmic approach to the synthesis of HENs was provided by Furman and Sahinidis [17]. An extended reviews about retrospectives on optimisation was given by Biegler and Grossmann [44[•]] and Grossmann and Biegler [45[•]]. They have been followed by Grossmann and Guillén-Gosálbez [46[•]] highlighting the main optimisation approaches in process synthesis and supply-chain management, and Friedler [47[•]] and followed by the update version [48^{••}] reviewing PA for energy savings and pollution reduction.

Targets and Heat Exchanger Network design

Setting targets for HI was widely publicised by Linnhoff *et al.* [4^{••}], followed by Smith in a series of his book, an early work Smith [31], the Russian version [32[•]] and so far the most recent book [33^{••}]. The second edition of Linnhoff *et al.* [5[•]] was elaborated on by Kemp [49^{••}]. A very good analysis has been developed by Gundersen [50^{••}] in his chapter of the PI Handbook edited by Klemeš [11^{••}]. Gundersen [50^{••}] summarised the important elements in basic PA as:

- (a) Performance Targets ahead of design,
- (b) The Composite Curves (CC) representation (Figure 1) can be used whenever an ‘amount’ (such as heat) has a ‘quality’ (such as temperature), and

Figure 1



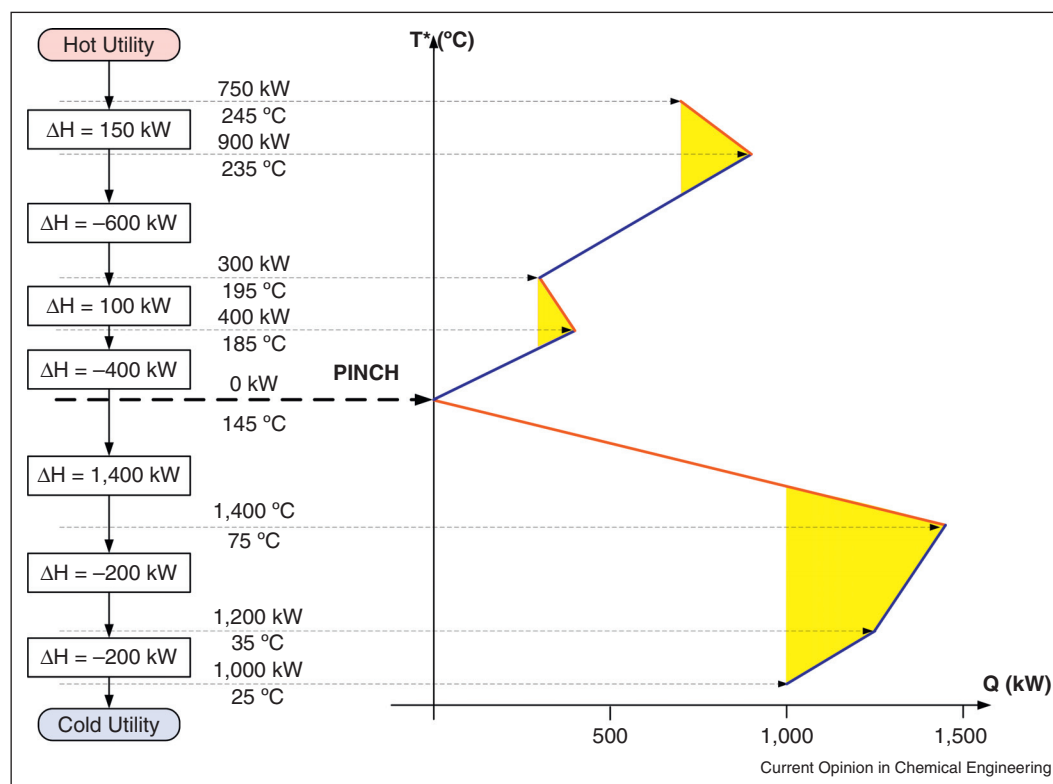
Composite Curves showing Heat Integration (developed from [130[•]]).

- (c) The fundamental Pinch Decomposition into a heat deficit region and a heat surplus region.

Heat recovery between hot and cold streams is restricted by the shapes of the CCs and the fact that heat can only be transferred from higher to lower temperatures. The minimum allowed temperature difference (ΔT_{\min}) is an economic parameter that indicates a near-optimal trade-off between investment cost (Heat Exchangers-HE) and operating cost (energy). The point of smallest vertical distance (equal to ΔT_{\min}) between the CCs represents a bottleneck for heat-recovery and is referred to as the Heat Recovery Pinch. An alternative representation of the overall heating and cooling demands within a process is the Heat Cascade (Figure 2, left), a special case of the transshipment model from Operations Research. Hot streams (heat sources) contribute to a set of temperature intervals (‘warehouses’ of heat), whilst cold streams (heat sinks) draw heat from the same intervals. The temperature intervals are established on the basis of the supply and target temperatures of all process streams. A heat balance is made for each temperature interval, and any heat surplus from that interval is cascaded (thus the name) down to the next interval with lower temperatures. The Heat Cascade also forms the basis of the Grand Composite Curve (GCC) — Figure 2, right, also referred to as the Heat Surplus Diagram, a very important tool for studying the interface between the process and the utility system (consumption and generation of various types of utilities, both load and level) and for evaluating the HI of special equipment into the process schemes.

The important property of the Heat Recovery Pinch is that it decomposes the process into a heat deficit region Above Pinch and a heat surplus region Below Pinch. On the basis of this insight about Pinch Decomposition,

Figure 2



The Heat Cascade and the Grand Composite Curve (developed from [77]).

systematic, step-wise design procedures have been developed for HENs with minimum energy consumption.

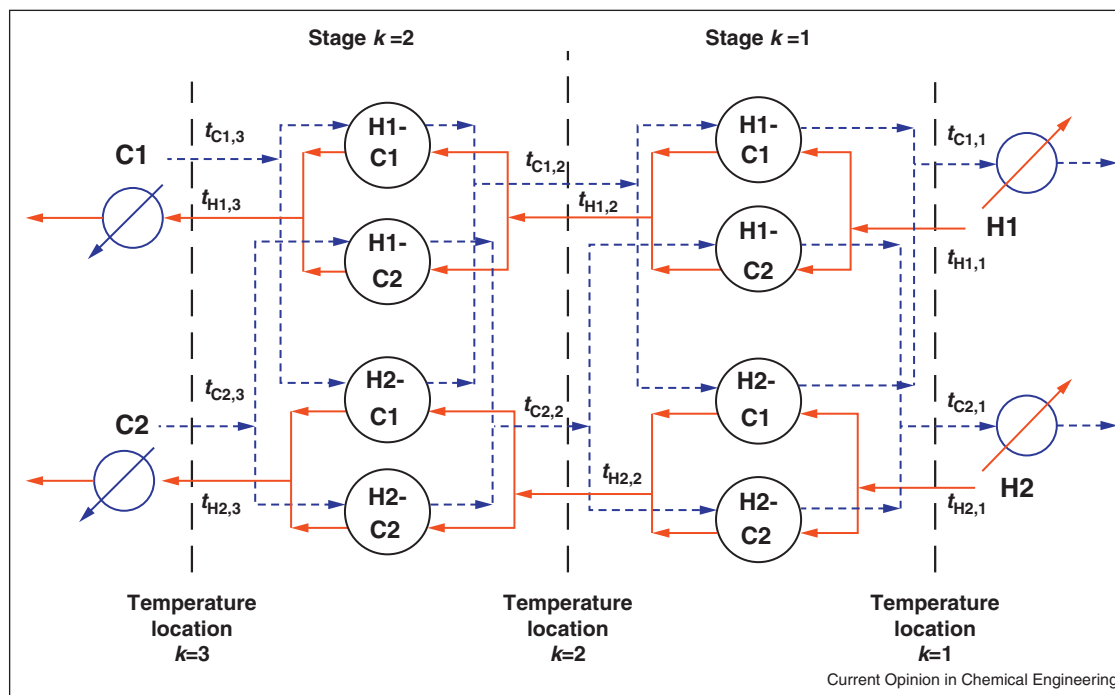
The earlier attempts in MP relating to HI were directed towards the development of models for predicting the minimum consumption of utilities and the minimum utility cost [41[•]]. For more advanced tasks, an expanded transshipment or transportation model with constrained matches [51] can be used for forbidding or forcing heat exchange between certain process streams. The latter is a typical example of achieving the feasibilities of constrained design problems, which would require an extension of the Problem Table. The important advantage of these HI models is that for the fixed temperatures and variable flows of the process streams they can be merged with process models to perform HI simultaneously with process optimisation. Some works have allowed for treating temperatures as optimisation variables — Papoulias and Grossmann [52[•]] used a discretisation scheme and Mixed Integer Linear Programming (MILP), while Duran and Grossmann [53^{••}] treated the temperatures in their Non Linear Programming (NLP) model as continuous variables. This model has been successfully used for almost four decades in equation-oriented process optimisations, as in the article of Duran and Grossmann [53^{••}], and modular simulators [42^{••}].

Analysis and design of heat-recovery systems for grassroots and retrofit situations

Most projects under the current economic situation have been devoted to upgrading the existing facilities, which includes retrofitting rather than the designing of new plants (so-called grassroots design). In order to boost the economic benefits of retrofit projects they are frequently combined with other process improvements. This dilutes the effect of plant downtime and the incentive and payback for retrofit projects can be considerably improved. However already Zhelev *et al.* [54] raised the issue of the need of HEN's operability analysis for better process integrated retrofit.

The MP approach was primarily oriented towards designing heat recovery systems for grassroots and later also for retrofit situations. The optimisation of HENs has probably attracted the most attention starting with the development of a sequential procedure for the synthesis of HEN consisting of three steps, namely the above-mentioned minimisation of utility consumption, minimisation of the number of matches at fixed consumptions of utilities [41[•]], as obtained in the first step, and finally the minimisation of area cost for exchangers [55[•]], as identified in the second step. In order to establish appropriate trade-offs between utility cost and investment, the

Figure 3



Stage-wise superstructure of HEN for two hot and two cold streams (after [57**]).

simultaneous NLP model for the area and energy targeting of HEN [56**], the Mixed Integer Non Linear Programming (MINLP) model for the synthesis of HEN [57**], and the MINLP model for simultaneous HEN synthesis and process optimisation [58**], were developed soon after the sequential procedure. It is interesting to note that those models do not rely on the concept of the Pinch temperature and the Heat Recovery Approach Temperature (HRAT) but on the selection of matches from the stage-wise HEN superstructure (Figure 3) where, for each stage, each hot stream can match any cold stream and all the temperature driving forces are regarded as optimisation variables. Different design constraints such as forbidden or required matches can be imposed. The model was extended for shell and tube heat exchangers, accounting for the pressure drops [59], and the heat transfer coefficients were determined from the shell and tube HE's design variables. Mizutani *et al.* [60] also performed HEN optimisation based on the trade-off between the heat transfer area and pumping cost. Besides double-pipe HE, other exchanger types can be embedded within the superstructure too; for example shell-and-tube, and plate and frame HE [61*]. The thermal design method for multi-stream heat exchangers of the plate and fin type was presented by Picon-Nunez *et al.* [62]. Nemet *et al.* [63] analysed important issues related to economy retrofit - the minimisation of a heat exchanger networks' cost over its entire lifetime.

Varbanov *et al.* [64*] approached the targeting the capital cost of TS recovery. For more recent developments in the area of HEN synthesis please refer to Klemeš *et al.* [65*].

The mentioned HI models for MP were later modified into HEN retrofit models. Ciric and Floudas [66], based on the transshipment model by Papoulias and Grossmann [41*], developed an MINLP model allowing for the retrofit and relocation of existing HE units. Yee and Grossmann [67*] extended their synthesis model [57**] for the retrofit of HEN. A two-step approach by [68] used constant approach temperature during the initial step and then MINLP to finalise the design during the second step. A combined MP and PA approach was proposed by Zhu and Asante [69*]. Accounting for different types of exchanges, Soršak and Kravanja [70**] extended their synthesis model [61*] for HEN retrofit. Mejia-Suarez *et al.* [71] developed a methodology for facilitating the search for good alternative retrofit solutions. Zhu *et al.* [72] developed a PA based approach and later Pan *et al.* [73] proposed a MILP-based optimisation method for retrofitting HENs with intensified heat-transfer. Zhang and Rangaiah [74] have employed integrated differential evolution (IDE) in order to perform discrete and continuous optimisation during the retrofit of HEN. Finally, Pan *et al.* [75] exploited tube inserts to intensify heat-transfer for the retrofit of HEN.

Application of HI to the synthesis of different systems

The Pinch design concept is very important not only because it contributed significantly to the efficient design of HEN but although because it provided important insights about the appropriate integration of energy intensive equipment into process schemes. As in the region Above Pinch we deal with heat deficit and Below Pinch with heat source, it follows that equipment requiring heat should be placed below and equipment releasing heat above it. Different rules for the placement of special equipment with respect to the Pinch were developed this way — for distillation columns [76], evaporators, heat pumps and heat engines [77], exothermic and endothermic reactors [78].

In the MP approach those rules were, however, considered indirectly by performing the simultaneous HI and the synthesis of corresponding systems: firstly, utility systems, for example a multistage refrigeration system by Shelton and Grossmann [79] and redone with the simultaneous HI by Kravanja and Grossmann [80], secondly, sequences of distillation columns, for example for sharp and non-sharp distillation by Aggarwal and Floudas [81] or for compact superstructures by Novak *et al.* [82], thirdly, reactor networks, for example a differential side-stream reactor model accompanied by coolers and heaters by Balakrishna and Biegler [83], and fourthly, overall process systems, for example the synthesis of the HDA toluene process by Kocis and Grossmann [84] and redone with the simultaneous HI by Kravanja and Grossmann [85]. Note that in more advanced applications the simultaneous synthesis of a system and Heat Integration can be performed via the synthesis of heat-integrated HEN, as was the case in the HDA toluene example [85].

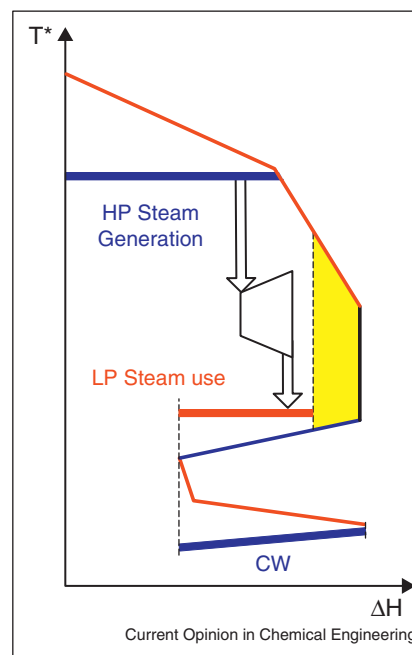
In the following subsections a more detailed review is provided for the heat and power utility systems as ones of the core systems regarding the applications of HI.

Application of HI to the synthesis of heat and power utility systems

The initial studies considering power generation and Combined Heat and Power (CHP) within the context of PI have dealt with the appropriate placements of heat engines relative to the heat recovery targets for a single process [77,86]. There are two cases — that of gas turbines and internal combustion engines, and that of steam turbines. They differ in their energy interfaces with industrial processes — gas turbines are net suppliers of high-temperature heat, whilst steam turbines both draw and reject heat at different temperature levels.

Integrating a steam turbine across the Pinch is equivalent to a Cross-Pinch heat transfer and results in a simultaneous increase of hot and cold utilities and an excessive

Figure 4



Exploiting a GCC pocket for extended co-generation (after [36]).

investment for the utility exchangers. Heat engines should be integrated in one of two ways:

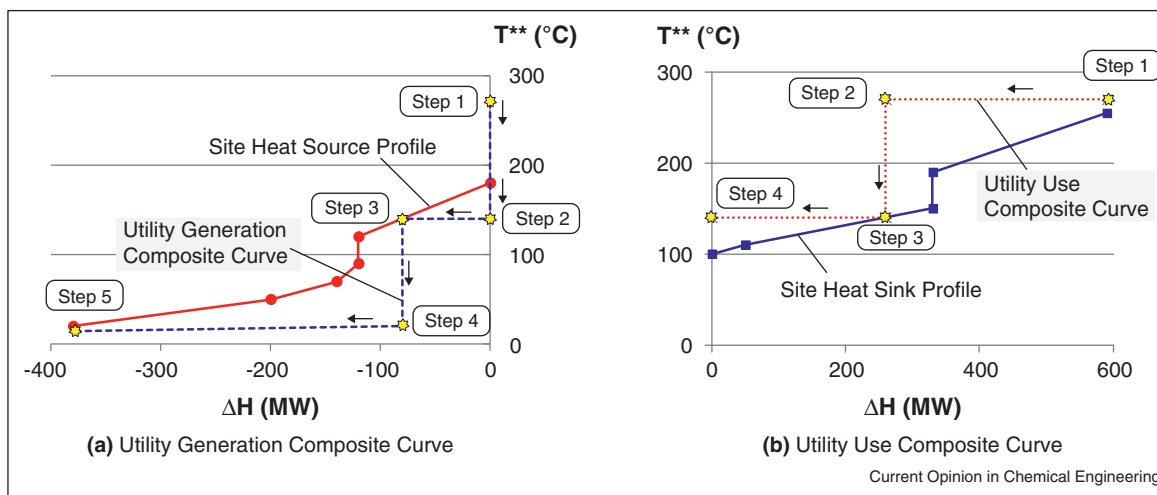
- Entirely Above the Pinch: this increases the hot utility by W for the main process but all the extra heat is converted into the shaft work.
- Entirely Below the Pinch: in this case the waste heat is used for power generation before rejecting the ambient.

One especially beneficial case of appropriate steam turbine placement is inside a GCC pocket (Figure 4), resulting in a 'free ride' [36]. However beside energy should be also, and in most cases predominantly is, considered the economy. The first issue to deal with are the prices. Even a seemingly small issues as 'What's the price of steam?' have not been always easy to answer [87].

Total Site Heat Integration

Higher-level HI can be performed using the site utility system for exchanging utilities. This is known as Total Site Heat Integration (TSHI) — first introduced by Dhole and Linnhoff [88]. The maximum possible heat recovery through a utility system can be targeted using the Site Sink and Source Profiles in combination with the steam header saturation temperatures. The source CCs for utility generation and use are constructed to account for feasible heat transfer from the Site Source Profile to the Site Source CC, and from the Site Sink CC to the Site Sink Profile. These curves are analogous to the individual

Figure 5



An example of construction of Site Source CC and Sink CC.

process CCs (Figure 5). The area where the curves touch is the Total Site Pinch [89^{••}] — usually confined to two steam levels (e.g. the MP and Low Pressure steam (LP) levels). The Pinching Steam mains feature is opposite the net steam loads. As with the Process Pinch, the Site Pinch divides an overall heat recovery problem into a net heat source and a net heat sink.

The work of Dhole and Linnhoff [88^{••}] was further developed by Raissi [90[•]] and extended by Klemeš *et al.* [89^{••}]. The latter paper describes the development of a tool called the Site Utility GCC (SUGCC). The area enclosed by this curve is proportional to the power cogeneration potential of the site steam system. Klemeš *et al.* [89^{••}] also defined a simple proportionality coefficient, the value of which is usually evaluated for each industrial site separately. This cogeneration targeting model is referred to as ‘the Temperature-Enthalpy (T-H) model’ because it is based on heat flows through the steam system.

Steam network synthesis

A steam turbine power generation model for the targeting, optimisation, and synthesis of steam turbine networks was developed by Mavromatis [91] initially for backpressure turbines. Its application to the design of steam turbine networks [92,93] included an improved cogeneration targeting procedure and was based on MILP. The steam turbine model was further extended by Shang [94] by accounting for condensing steam turbines. Shang [94] developed hardware models for fired steam boilers and gas turbines. He also provided a framework for steam level selection, superstructure construction, and optimisation of the resulting utility system’s configuration. A MILP trans-shipment formulation was used to obtain the

optimal steam header pressure levels. The difference from that of the earlier technique was that Shang [94] specified where to obtain the candidate pressures, based on the temperature boundaries of the site-level heat cascade (the kink points in the Site Heat Source and Sink Profiles). Aiming at the development of a robust framework for the optimisation of existing utility systems, Varbanov *et al.* [95] presented improved models for utility system components that account for all the significant performance factors in a systematic way. This procedure was further extended for tackling the problem of utility system synthesis [96[•]]. The developed synthesis method was later published in [97]. This method offers several fundamental improvements to the previous work in this arena:

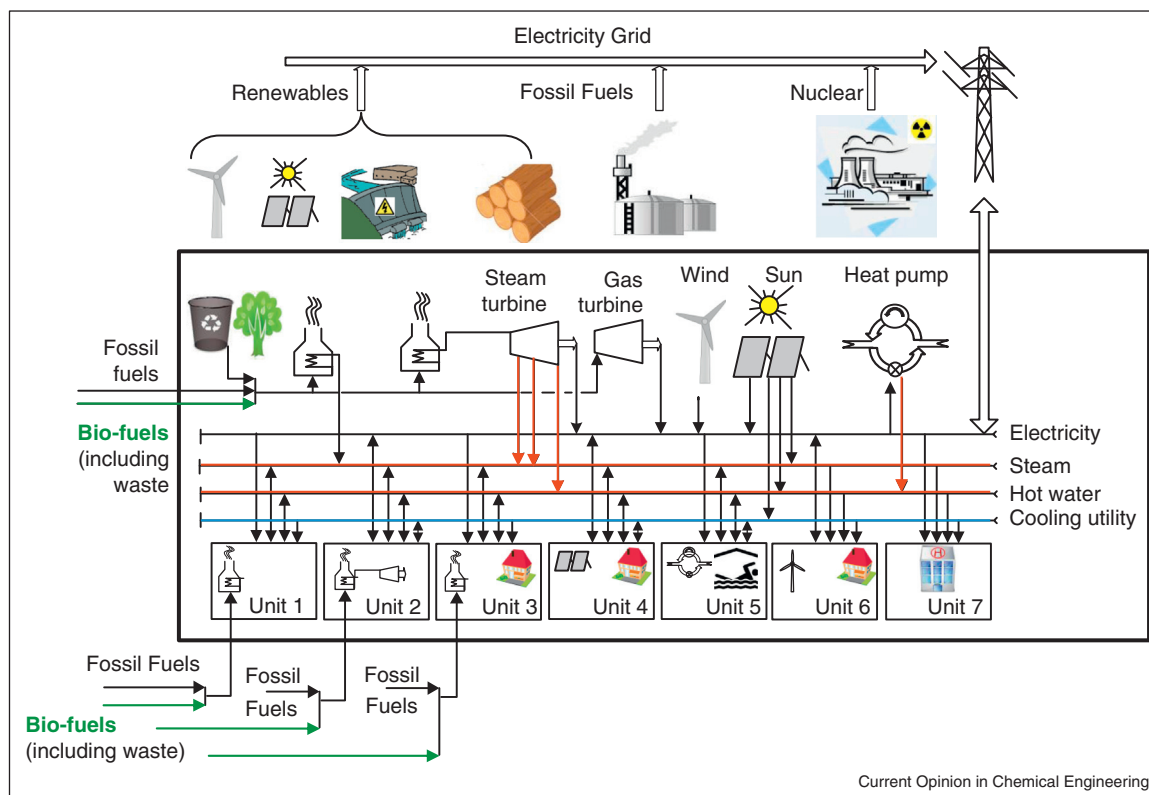
- Improved models of the utility system’s components.
- Improved optimisation framework using a successive MILP (SMILP) approach solution procedure.
- Integration of the emissions generation and costing into the overall system model.

Manesh *et al.* [98] applied an MINLP approach in combination with simulation using a STAR software environment (recent latest version is [99]) to one of the world’s largest deep water oil ports. Velasco-Garcia *et al.* [100] raised the issues of utility systems operation and optimisation of the decision making. Those issues should be considered for integrated steam systems.

Total Site Heat Integration (TSHI) methodology addressing varying energy supply and demand

For reduction of the carbon footprint from energy users, Perry *et al.* [101^{••}] conceptually extended the TSHI by integrating greater community servicing within residen-

Figure 6



Locally Integrated Energy Systems — an extension of TS HI.

tial areas, with service and business centres as additional heat sinks and renewable energy as heat-sources (Figure 6). The inherent variability in the heat supply and demand increased the difficulties in handling and controlling the system. This part has received considerable attention recently. Varbanov and Klemeš [102] introduced Time Slices into the Total Site (TS) description, with a heat storage system for accommodating the variations. Liew *et al.* [103] contributed with a numerical solution for the TSHI system by addressing the variables' availabilities. Nemet *et al.* [104] discussed the approaches needed for maximising the usages of renewable energy sources with fluctuating supplies. Varbanov *et al.* [105] revisited the global minimum temperature difference (ΔT_{\min}) used in the previous method. Liew *et al.* [103] introduced a numerical method known as the Total Site Problem Table Algorithm (TS-PTA) for targeting the TS utility requirement, intended to allow automation when obtaining the TS targets. Top-level analysis [96] is another mathematical modelling methodology that can be used for these concepts. This method allows for 'scoping', that is, selecting the site processes for targeting HI improvements. Chen *et al.* [106] proposed a systematic optimisation approach for designing a Steam Distribution Network (SDN) of steam systems in order to obtain an improved energy utilisation within the network. Bandyopadhyay *et al.*

[107] proposed a simplified methodology for targeting cogeneration potential based on the Salisbury [108] approximation. Kapil *et al.* [109] introduced a new model based on an isentropic expansion. Total Site Sensitivity Table (TSST) was proposed by Liew *et al.* [103]. This tool could be used to systematically determine the minimum and maximum boiler and cooling utilities' capacities under different operating conditions.

Conclusions — challenges and drivers

HI has been a leap forward in the development of resource conservation and emission reduction. Its crucial advantage has been the conceptual clarity and insight delivered to the practising engineers, which helped its widespread, fast, and robust adoption. Combining the conceptual insight with the power of MP has made HI even more robust and powerful in solving large-scale problems. The methodology is thriving even forty years after its conception.

Challenges and recent developments in MP, and the combined approach

Different directions in MP have been undertaken in order to overcome a number of drawbacks related to the use of MP, for example global optimisation in order to provide global solutions, the development of graphical interfaces

Table 1

Opportunities of employing a combined PA/MP approach in HI.

Approach	PA	MP	Combined
Guiding principle	Physical insights, Clear concepts — Targeting even before the design	Numerical Mathematics	Both principles could be employed narrowing the searching space of MP
Embedded principles	Consideration of physical laws	Optimality, feasibility, and integrality of solutions	Both principles are considered
A single criterion	Mainly technological criteria, for example minimal consumption of utilities in utility targeting relates to sustainability	Mainly economical criterion, for example total annual cost in HI process optimisation	Appropriate economic trade-offs can be obtained when both criteria are considered
Multi-criteria consideration	Difficult to express graphically, possible with PTA	Multi-objective Optimisation (MOO) can be performed for several criteria	Multi-criteria can be considered
Degrees of freedom	Difficult to express graphically, possible with PTA	Can handle a large number of optimisation variables	Large problems with large numbers of optimisation variables can be solved
Data collection and verification	The physical inside makes the checking easier	A possibility to apply data reconciliation algorithms	Combination can be very beneficial
Uncertain data and parameters	A number of scenarios with a some number of uncertain parameters, provides limited flexibility of solutions	A reasonable number of uncertain parameters simultaneously in order to obtain flexible solutions	Feasible, realistic and Flexible solutions can be obtained
Approach strategy	Can eliminate easily physically non feasible solutions, allows clear interaction of the designed between decision steps	Simultaneous (both-way interactions can be synergistically exploited) — fully integrated, for example simultaneously heat-integrated process flowsheets, but not easy to interact during the solution	By applying the both strategies in a sequence fully integrated solutions can be obtained
Problem formulation	Both graphical based on thermodynamic and algorithmic and form — easily understandable to designers	Usually Equation-Oriented (EO) mathematical form. Needs to collect full data set	Hybrid model formulation in order to simplify the EO formulation enabling solving larger-scale problems
Easiness of formulation	Straightforward and mostly easy	Could be very complicated Requires to consider all the options, some can be missed	Hybrid model formulation can be complicated, however Pinch is beneficial in the first step followed by MP
Easiness of problem reformulation	Very easy when supported by PTA	Many scenarios can be routinely performed if the problem is fully formulated	Pinch is again beneficial in the first step followed by MP
Optimality of solutions	Global optimal targets can be indicated based on the thermodynamics. Provides a number of close to global optima possibilities. How to reach those targets usually MP is needed	Unless global optimisation techniques are employed, the solutions are locally optimal and can be due to a presence of non-convexities far from global optima	Pinch concept can guide MP solutions close to global optima
Comprehension of solution	Straightforward, both with graphical methods and PTA Provides clear new insights	Numerical solutions are usually not easy to be interpreted New insights can be obtained from solutions	Combined graphical interfaces can be developed in order to support the mimic of MP solutions
Knowledge needed	Seems basic engineering, however needs a process expert	Advanced knowledge, both engineering and IT (mathematical)	Experienced Process engineer guaranties realistic solution for both approaches. For MP some IT (mathematical) support is a bonus
Robustness	Robust, which is important for engineering practice	LPs and MILPs are fairly robust while NLPs and MINLPs need good initialisations in order to get feasible solutions — can be provided by PA	Overall robustness in solving large-scale problems is improved by the synergy of both approaches
Current industrial acceptance	High, easily understandable to engineers on the ground	So far lower, should be boosted by engineering friendly interface	Could foster the acceptance of MP in process and other industries, especially if used in a sequence

to help users to comprehend their resulting numerical solutions, or the development of open source and generic data-independent models for providing users mathematical formulations for different current and future applications. Finally, different techniques and tools have been developed for solving complex industrial applications by using the advantages of the combined concept. As the PA and MP concepts exhibit different advantages and drawbacks, the important question is which of the drawbacks of the PA can be overcome by MP, and vice versa. However beside MP has been also other tools, which can be applied in HI as P-Graphs developed by Friedler *et al.* [110[•]], for an implementation see for example Varbanov and Friedler [111].

Table 1 presents some basic features of both approaches, as well as possible opportunities for employing the combined approach.

Challenges and recent developments in PA based HI

HI based on classical graphical tools and PA has been developing in various directions. It soon became obvious that it had very wide options regarding analogies to be harvested and beneficially used. They have been various challenges in directions and branches, which could never have been considered forty years ago.

However, when implementing HI and TS HI within industrial environments, some important issues should be considered when dealing with the model which is closest to reality [112[•]], and more recently Chew *et al.* [113[•]]. Another significant issue of HI especially important for TSHI dealing with the consideration of the site distance factor raised Wang *et al.* [114[•]]

A very important issue also stemming from Table 1 is the software tools. Several specialised HI tools are available. A short summary is available from Klemeš *et al.* [65[•]], more comprehensively from Bulatov [115[•]], and another overview was published by Lam *et al.* [116^{••}].

An important issue is also the teaching and training including higher education and further professional development courses. Several papers have been presented dealing with Information Technology (IT) tools Liew *et al.* [129], and also Grigorov *et al.* [117].

On TS methodology development: TS Sensitivity Analysis — Liew *et al.* [103[•]], Industrial implementation issues of TSHI — Chew *et al.* [113[•]], and Atkins *et al.* [118] PI between individual plants at a large dairy factory by the application of heat recovery loops and transient stream analysis. Including renewable energy sources and variation in supply and demand has been another direction of recent research — for more details see for example Varbanov and Klemeš [102[•]].

Gerber *et al.* [119] defined the optimal configurations of geothermal systems using process design and HI techniques. The problem of soft data in PI has been studied and industrially applied by Walmsley *et al.* [120]. An important issue that needs extended attention in HI problems as well as in the other developments of PI is data reconciliation [121[•]]. HI issues not covered in this overview, but still important are the targeting and designing of batch processes, see for example Foo *et al.* (2012) [122] and cost-effective HEN design for non-continuous processes by Morrison *et al.* [123[•]]. Most recent very good batch related paper dealing with Indirect Thermal Integration has been published by Chaturvedi and Bandyopadhyay [124[•]].

On TSHI until recently heating (steam and hot water) and cooling (water, air and refrigeration) have been mainly considered. This has been recently extended into power/electricity by the works of Wan Alwi *et al.* [125[•]] dealing with a PI Targeting Method for Hybrid Power Systems, Mohammad Rozali *et al.* [126[•]] providing a methodology for PI techniques for the optimal designing of hybrid power systems and Ho *et al.* [127] combined design and load shifting for distributed energy system.

The more recent overviews of PI have in most cases been related to sustainability, they include Klemeš *et al.* [36^{••}] — Sustainability in the Process Industry–Integration and Optimisation, El-Halwagi [10^{••}] — Sustainable Design through PI–Fundamentals and Applications for Industrial Pollution Prevention, Resource Conservation, and Profitability Enhancement, Foo [128^{••}] — PI for Resource Conservation and more recently by an editing Handbook on PI to which most of the leading researchers contributed [11^{••}].

This list is cannot be fully comprehensive, but very substantial research results are being publishing virtually every week. This can be continued and its growth accelerated. This provides very strong evidence that PI methodologies, based on both Pinch and MP have still not reached their saturation points and many extensions are still to be envisaged.

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