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Process integration, modelling and optimisation for energy saving and pollution reduction

Ferenc Friedler*

Faculty of Information Technology, University of Pannonia, Egyetem utca 10, H -8200 Veszprém, Hungary

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ABSTRACT

Energy saving, global warming and greenhouse gas emissions have become major technological, societal, and political issues. Being closely related to energy supply, they are of a strategic importance. Various conferences are being organised for providing international venues for closer cooperation among researchers. The series of conferences "Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction" (PRES) play a pioneering role in contributing to the solution of the related problems through presenting new methodologies and initiating cooperation among participants that often result in international projects. The PRES conferences have been dedicated both to the theoretical and to the practical aspects of energy saving and pollution reduction. The PRES series, established thirteen years ago, was originally dedicated to energy integration and improving thermal efficiency. Following the new challenges and priorities, the scope of the conferences has been extended to include all energy and pollution prevention related issues. This contribution focuses on the period covered by PRES, reviewing at least some major presentations contributing to the development of process integration and optimisation tools for energy saving and pollution reduction. The development of the mathematical models has been covered as well, since it is closely related to the area.

1. Process integration (PI)

PI is a family of methodologies for combining several processes to reduce consumption of resources or harmful emissions to the environment. It started as mainly heat integration stimulated by the energy crisis in the 1970's.

1.1. Early stages of PI

It is remarkable that PI has not lost the interest of researchers for nearly 40 years and even has been flourishing recently. One of the first related works was that by Hohmann [1] in his PhD thesis. He has not pursued the research any further and in that "ancient pre-internet age" its enormous potential has not been recognised by the research community at that time. It was Bodo Linnhoff and his PhD supervisor the late John Flower at University of Leeds who continued this work. They used Hohmann's work and in 1977 developed the basis of pinch technology, which is now considered as the foundation of heat integration. As usual in case of a pioneering innovation, it was difficult to publish. The first publication appeared in 1978 [2] due to their strong commitment. This has become one of most cited papers in the history of chemical engineering. A similar work has been done in Japan more or less in parallel [3,4]. However, it was again Linnhoff who pushed the new concept through the academia and the industry. An important step was his arrival, via an industrial appointment at ICI Ltd in Runcorn, Cheshire, to that time UMIST where he set up the Centre for Process Integration and the Process Integration Research Consortium.

1.2. Pinch technology for heat integration

The publication of the first "red" book by Linnhoff et al. [5] played a key role in the dissemination of heat integration. The book received a new extended Foreword reflecting the up to date developments. It has been again massively cited in the literature and is considered as the first overview of the area. This User Guide through pinch analysis provided insight into the most common process network design problems including heat exchanger network synthesis, heat recovery targeting, and selecting multiple utilities. Heat recovery targeting is based on the Composite Curves (CCs) [6]. This is a visual tool, providing important energy-related properties of an industrial process in a single view. The overlap between the curves represents the heat recovery target, while the minimal needs for external heating and cooling are represented by

* Tel.: +36 88 424 483; fax: +36 88 428 275.
E-mail address: friedler@dcs.uni-pannon.hu.

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the non-overlapping segments of the cold and hot composite curves, respectively. Most importantly, these thermodynamically derived heat recovery targets cannot be exceeded by any real system. CCs play an important role in process design. For direct Heat Exchanger Network (HEN) synthesis algorithms, they provide strict targets for Maximum Energy Recovery (MER). For process synthesis based on Mathematical Programming or combinatorics, they provide relevant lower bounds on utility requirements and capital cost, narrowing the search space of the optimisation. The recognition of the thermodynamic limitations and relationships in the underlying heat recovery problem has led to the development of the Pinch Design Method [7]. This method is capable of producing maximum heat recovery networks.

A further development for Heat Integration targeting has been the Grand Composite Curve — GCC [8], together with the associated Heat Cascade and the Problem Table Algorithm [2]. The GCC shows a clearer view of the areas of internal process heat self-sufficiency as well as the demands for external heating and cooling — all in the context of the corresponding temperature levels. The appropriate combination of utilities can be targeted aiming at minimal emissions and/or utility cost.

1.3. Mass and water pinch

Inspired by the success of Heat Integration, researchers have spread the Pinch idea to other areas — in particular to mass exchange [9]. Wang and Smith [10] developed a synthesis method for industrial Water Networks as a special case of Mass Exchange Networks. The main objective was to simultaneously minimise the consumption of fresh water and the disposal of wastewater by maximising the internal water reuse. Wastewater generation can be further reduced by applying water regeneration, allowing further reuse or recycling. For cases of single-contaminant problems, translating the Pinch Analysis to water minimisation is straightforward, constructing the composite curve of water use as a plot of the contaminant concentration versus contaminant load. Extending the Water Pinch Analysis to multiple-contaminant problems, however, is complicated and difficult to use. The major issue is which contaminant is selected and used for plotting the composite curves. Many approaches are available. One useful option is to employ Mathematical Programming; where Water Pinch serves as a preliminary scoping and visualisation tool.

1.4. Other pinch based methodologies

The Pinch Principle has also been applied to other types of processes and areas, the most prominent being Total Site Integration, refinery hydrogen management, Carbon Footprint estimation/minimisation, and wastewater treatment.

1.4.1. Hydrogen pinch

Previously hydrogen availability was not a problem for refineries, but several new trends have caused an increased demand for hydrogen. A methodology has been developed for assessing the available hydrogen resources on a site, using the so-called Hydrogen Pinch Analysis [11]. It constructs Hydrogen Composite Curves accounting for the demands and sources of hydrogen on a site in terms of stream purity versus flowrate. That is used to construct a hydrogen surplus diagram similar to the GCC in Heat Integration. These instruments allow engineers to find the system Hydrogen pinch and set targets for hydrogen recovery, production and import by a refinery. This methodology has been improved by Hallale and Liu [12] accounting for pressure as a factor and, therefore, making the best use of the existing compressors in the refinery. This improved method can also account for important costs and tradeoffs including hydrogen production, compressors, fuel, and piping costs.

1.4.2. Oxygen pinch

The strive to design more cost efficient waste treatment systems inspired yet another extension of the pinch principle — the Oxygen Pinch Analysis [13]. The idea was to target prior to design the ideal minimum oxygen demands for micro-organisms aeration. Flowsheet and design changes were suggested based on the target. Agitation and other forms of aeration require energy, so finally, the analysis based on oxygen pinch principles leads again to their original application associated with energy conservation. The method also provides other indicators — quantitative targets for oxygen solubility, residence time, and oxidation energy load. In a follow-up development, a combined Water and Oxygen Pinch Analysis has been proposed [14]. By combining the two criteria, up to 30% cost savings for the wastewater treatment could be achieved.

1.4.3. Total site

To develop a good understanding of industrial energy systems, a graphical method has been developed based on the concept of the Total Site [15]. This introduced the concept of the site's heat source and heat sink profiles. By integrating a number of processes via the steam system, additional inter-process heat recovery can be achieved by using the total site profiles as guides. The method allows a target to be set for the total site heat recovery. Data for process heat recovery are first converted to grand composite curves (GCCs). The pockets of the GCCs representing the scope for process to process heat recovery are removed and the modified GCCs are combined to form a site heat source profile and a site heat sink profile. The sink and source profiles are superimposed on the steam header saturation temperatures and CC of steam generation and usage are constructed, accounting for feasible heat transfer from the heat source profile to the steam generation composite and from the steam usage composite to the heat sink profile. The work by Dhole and Linnhoff [15] and by Raissi [16] was further developed by Klemeš et al. [17]. On the basis of the Steam Composite Curves, thermodynamic targets for heat and power cogeneration can be set. The cogeneration targeting model has been further refined and improved by Mavromatis and Kokossis [18], later by Varbanov et al. [19] and the most recently by Varbanov and Klemeš [20].

1.5. Contributions of PRES conferences

1.5.1. First PRES conferences PRES'98 and PRES'99

PRES Conferences contributed considerably to the development of PI methodologies and dissemination of successful case studies. Bodo Linnhoff presented one of his last plenary lectures [21] on the automated interface between simulation and integration. This has been a substantial step towards data extraction for PI software tools. The plenary has been rather comprehensive and suggested the way forward for this important task. The problem received some interest during the following years and several software packages have been offering support for this task. Despite this, more work should be done to satisfy the needs for industrial applications. Recent trends in PI, software and applications were presented by Gundersen [22]. He proclaimed an important development of Hybrid PI methods created by merging previously competing schools — Pinch Technology and Mathematical programming. Bochenek et al. [23] compared retrofitting of flexible HENs by optimisation versus simulation approach. This has been very important work in the field which still deserves more research. Zhu et al. [24] proposed heat transfer enhancement for HEN retrofit design, from which Heat Integration can substantially benefit. This methodology still deserves wider implementation especially for retrofit studies. Hassan et al. [25] presented a successful PI analysis and retrofit suggestions for an FCC plant. It is one of the first comprehensive retrofit case studies. Kalitventzeff et al. [26] covered the usefulness of PI in the application to the isothermal gas turbine. Plesu et al. [27] demonstrated the wide applicability of PI in the Romanian oil refining and petrochemical industry. Klemeš et al. [28], made a series of applications of Pinch technology in the food industry. This has been further developed in [29]. They had shown that Pinch technology can provide benefits far beyond oil-refining and petrochemicals. Mařík et al. [30] presented a design tool for flexible and energy-efficient HENs. This approach has been based on an expert system and optimisation. The PRES'99 forum was held in Budapest - Hungary. It has been a major step in the development of the conference — both in terms of the number of participants and in the scope of covered areas. In the plenary lecture Smith [31] made an overview of Process Integration. Zhu and Vaideeswaran [32] reviewed an extension of the Total Site methodology — the Top Level Analysis. This approach has considerable potential, part of which has been realised with its efficient optimisation-based computational implementation by Varbanov et al. [33]. Fraser and Hallale [34] attempted effluent reduction through pinch technology and demonstrated it on gold solvent extraction plant. Interesting extension was also an impact diagram showing effluent reduction versus capital investment target. Hashemi-Ahmady et al. [35] came up with a sequential Framework for Optimal Synthesis of Industrial HENs by combining Pinch Analysis and simultaneous MINLP methods. The idea has been further developed at following PRES conferences. Zhelev and Bhaw [36] introduced an Oxygen Pinch Analysis and combined it with water Pinch Analysis for wastewater management. Klemeš et al. [37] summarised a comprehensive experience of retrofitting Polish Sugar Factories using PI. They presented the implementation of Heat Integration up to Total Site level considering retrofit features in combination with process modifications, based on close collaboration with the staff from the factories. Aaltola [38] suggested through case studies the integration of a paper mill with two sites district heating including seasonal variations. However, at that stage several important issues have been just drafted and opened for the future research. Another case study dealt with heat and exergy analysis of biomass fuelled integrated gasification humid air turbine – BIO-IGHAT plant [39]. This is a new class of problems simultaneously applying heat integration and exergy analysis. Dogru et al. [40] performed a case study – using a software tool from Linnhoff March [41] for an ammonia plant. However, the analysis covered just the first step and did not continue into advanced heat integration steps. Galli and Cerda [42] adopted an approach based on MINLP for the synthesis of HENs featuring a minimum number of bounded-size shells. Their approach would benefit from its combination with Process Integration. Rodera and Bagajewicz [43] suggested a heat integration approach across plants using multipurpose heat exchangers. They extended the Minimum Matching Approach of Papoulias and Grossmann [44]. Their targeting procedure has been further developed. Gottschalk et al. [45] applied a Heat Integration Expert System for energy integration of industrial chemical processes. Their interesting feature was the combination with Pinch technology, which was demonstrated on an industrial case study for the synthesis of Methyl-tert-butyl-ether. This approach has still a good potential to be explored further. A well developed industrial case study was presented by Markowski [46] — a retrofit of crude distillation unit. He covered important features of fouling and brought this case study close to the industrial conditions. Seikova et al. [47] presented a retrofit debottlenecking of a heat integrated crude oil distillation system building upon previous works of the UMIST team [48] as well as on the approach presented by Varbanov and Klemeš [49,50]. Tovazhyansky et al. [51] used the heat integration methodology spread by the collaboration with UMIST under the UK Know-How Fund to district heating, chemical industry, ammonia plants, and food and drink industry across Ukraine.

1.5.2. PRES 2000

Kalitventzeff et al. [52,53] emphasised that better solutions can be generated for process sustainability through process energy integration. They shared their experience in the implementation of process energy integration techniques and their contribution to the process sustainability in an ammonia plant including combined production of heat and mechanical power for an existing process. Pinch technology and its recent extensions offer an effective and practical method for designing the HEN for new and retrofit projects. Al-Riyami et al. [54,55] demonstrated a heat integration retrofit analysis of a HEN of a fluid catalytic cracking (FCC) plant. The study found significant scope for improvement in the heat recovery. The new network was designed using the network pinch method. Grabowski et al. [56] presented a case study of energy minimisation in sugar production by applying PI. The minimum energy consumption of the process was determined by simultaneous energy targeting and optimisation of evaporation. Energy systems employing various CHP technologies and various evaporator stations optionally combined with vapour compressors have been studied. A range of feasible solutions has been defined in terms of minimum energy consumption and combined heat transfer area of the evaporator station and the HEN.

1.5.3. PRES'01

Sadhukhan and Zhu [57] examined the integration of gas technologies in the context of overall refinery in order to use gasification for stretching the economic margins to the full extent. A stage-wise optimisation strategy was developed in order to capture interactions among refinery processes, the gasification system and hydrogen and utility networks. Integration of waste to energy is a good option for thermal processing of waste. Bébar et al. [58] demonstrated the method of efficiently utilising the heat value of the incineration products and thus partially compensate the costs of waste thermal treatment. Cheung et al. [59] addressed another important aspect in PI. They presented the Total Site Maintenance Scheduling for better energy utilisation. To minimise the impacts on production and utility systems during routine maintenance the scheduling has to be done carefully with consideration of site-wide utilities and material balances.

1.5.4. PRES 2002

Smith [60] highlighted the advantages of PI for reduced environmental impact in his plenary lecture. He pointed out that PI techniques have been extended beyond their original scope for solving energy problems to be able to address a wide range of process design issues. Rodera et al. [61] presented a contribution to PI methodology for improving HEN operation. Their methodology featured a workflow to assist in the analysis of an existing HEN design when the operating conditions vary. It facilitated the involvement of the engineer in the daily operation and maintenance of the network. A method to target the optimal integration of the utility system was demonstrated by Marechal and Kalitvenzeff [62,63]. They addressed multi-period optimisation incorporating models for selecting and targeting the optimal operation strategy of the utility system. This includes gas turbines, steam network and cooling system together with the calculation of the optimal heat recovery system. Václavek et al. [64] studied pressure as another parameter of the composite curves in heat integration. An important attempt has been made to evaluate the importance of pressure in heat integration. Cost estimation can have a major impact on project profitability. Taal et al. [65] provided a summary of the common methods used for cost estimation of heat exchange equipments and the sources of energy price projections. It shows the relevance of the choice of the right method and a reliable source of energy price forecast used when choosing between alternative retrofit projects or when trying to determine the viability of a retrofit project.

1.5.5. PRES'03

In an important extension of PI methodology the total site idea was applied by Sorin and Hammache [66] using a new model for shaftwork targeting. A modified Site Utility Grand Composite Curve (SUGCC) diagram was proposed. The new model allows targeting fuel consumption, cooling requirement, and shaftwork production with high accuracy and visualising them directly as special segments on the T–H diagram. The concept of thermal integration of trigeneration systems was presented by Teopa Calva et al. [67]. The use of the thermodynamic model helps simulating the main components of the system and permits a fast and interactive way to design the optimum trigeneration scheme using the performance data of commercial gas turbines. Lavric et al. [68,69] presented the benefits and drawbacks of energy integration through virtual heat exchanges. The features of the proposed Reactors Energy Integration were illustrated by a case study, a two-bed methanol synthesis heat integrated reactor. Brown et al. [70,71] have combined Pinch Analysis, exergy analysis, and optimisation techniques to define energy targets at pulp and paper industry expressed in terms of the energy costs rather than energy requirements. The dual representation of thermodynamic and technological energy requirements can be a valuable tool for the early stages of process energy analysis. PI approach was extended to water network design. Foo et al. [72,73] applied the water pinch analysis to synthesise maximum water recovery networks for batch processes. A new numerical technique, time-dependent water cascade analysis was demonstrated. This new network representation has an advantage of clearly depicting the time-dependent nature of a batch water network. Majozi [74] presented an effective technique for wastewater minimisation in batch processes by formulation of a MINLP mathematical model approach. This water integration work minimised wastewater production through the implementation of numerous recycle and reuse opportunities. An extended Pinch Technology was proposed by Zhelev [75] to deal with water and energy management. The application of the methodology is designed to achieve water conservation through minimisation of evaporation losses. Its significance was demonstrated through case studies of a power station, a brewery, and a tissue factory.

1.5.6. PRES 2004

Kaggerud et al. [76] suggested a new avenue of PI combined with chemical integration. Process and chemical integration is proposed as an option to increase the overall efficiency as co-production of power and chemicals is utilised. Chemical and PI can give economy of scale savings, better utilisation of the raw materials, improved energy efficiency and savings in investment costs. Another heat integration contribution was presented by Anantharaman et al. [77]. Pinch Analysis, Exergy Analysis and Optimisation have all been used independently or in combination for the energy integration of process plants. Cziner et al. [78] addressed the potential of multi-criteria, performance decision-making in plant design with the aid of PI. A hierarchical decision-making methodology was presented, where the environmental and safety regulations and the growing demand of consumers for higher product quality are included. The case study had a calcinations kiln, followed by flue gas cleaning and heat recovery systems.

The Pinch principle was further extended by Zhelev [75] in the opportunities to improve profits and reduce the investment cost through integrated management of resources such as electrical energy, steam and fresh water. Cost Composite Curves were created to target the optimum profitability to guide the decision-making process in the context of key tradeoffs. A Grid diagram analogy was used to show the money flow that can ensure meeting the targets.

1.5.7. PRES'05

Based on Pinch Analysis, a procedure was proposed by Markowski et al. [79] for minimising the compressor shaft work in the refrigeration system. They studied the thermal separation of hydrocarbon mixtures in a sequence of heat-integrated distillation columns coupled with a refrigeration system via a HEN. An automated approach for heat integration was presented by Moodley et al. [80]. They used a superstructure and a mathematical model to demonstrate the optimum cooling water supply to a network of heat exchangers supplied by multiple sources. The concept of comprehensive PI was introduced by Hurme et al. [81]. It was defined as design, operation and management of industrial processes with system-oriented and integrated methods, models, and tools. Mascia and Majozi [82] presented an industrial case study on the synthesis of partially thermally coupled and heat-integrated distillation systems applied to the light ends separation section of a crude distillation plant. This distillation system employs the thermal coupling and the heat integration principles to significantly reduce the heat requirements compared with the traditional simple column train. Picón-Núñez et al. [83] studied the effect of the configuration of cooling networks on the total exchanger area. The chosen methodology combined the pinch design method based on vertical heat transfer and the minimum-water-use design method. A case study demonstrated the methodology showing a practical approach to reduce operating costs in existing systems. An extended pinch analysis and design procedure evaluating pressure based exergy for sub ambient cooling were presented by Aspelund et al. [84]. They demonstrated a substantial potential for minimising energy requirements (total shaftwork) in subambient processes. The compression and expansion work is optimized for the process streams, together with the work needed to create necessary cooling utilities.

Panjeshahi and Tahouni [85] presented the method of Pressure Drop Optimisation in Debottlenecking of HENs. Their method had been effectively applied in a case study involving the retrofit of a crude oil pre-heat train after increasing throughput. The debottlenecking of HENs using optimum pressure drops would be able to predict the required additional heat recovery area with acceptable accuracy. Lior [86] reviewed the status and prospects of using fossil, nuclear and renewable energy for power generation (including hydrogen, fuel cells, micropower systems, and the futuristic concept of generating power in space for terrestrial use). He summarised the promising energy R&D areas, their potential, foreseen improvements, their timescale, and latest trends in government funding.

1.5.8. PRES'07

The Pinch Technology was extended to CO_2 minimisation. Foo et al. [87,88] demonstrated a Cascade Analysis Technique for Carbon and Footprint-Constrained Energy Planning. They presented algebraic targeting techniques for energy sector planning with carbon (CO_2) emission and land availability constraints. Cirlly and Zhelev [89,90] presented a pinch analysis for CO_2 emissions targeting and planning, accounting for the dynamic nature of electricity supply–demand. Amann et al. [91] presented the conversion of a natural gas combined cycle power plant using an advanced gas turbine for CO_2 pre-combustion capture. CO_2

recovery rate has a big impact on the power plant efficiency since a lot of steam is required to lower the low heating value of the synthesis gas leaving the recovery process, thus reducing NO_x. Perry et al. [92,93] extended the total site approach to integrate waste and renewable energy to reduce the carbon footprint of locally integrated energy sectors. This novel method can be successfully applied to integrate renewables into the energy source mix and consequently reduce the CFP of these locally integrated energy sectors. Liebmann et al. [94] evaluated different scenarios of bioethanol production with innovative energy supply facilities. They studied the options for renewable energy supply such as biogass applied for CHP and biogas boiler. This gave a good start to the integration of renewable energy into regional energy supply.

Foo et al. [95] paid attention to heat integration in batch processes. Their work covered the minimum units targeting and network evolution for batch HENs. The minimum units target sets the lower bound for a batch HEN prior to the network evolution, which is used to evolve the network to reduce its complexity. They have shown that to simplify a batch HEN with network evolution techniques, a thorough analysis has to be performed across all time intervals of the batch process. Two examples illustrated the applicability of the proposed techniques. Further work is envisaged by them to incorporate the targeting and evolutionary techniques into a rigorous optimisation model.

1.5.9. PRES 2008

Klemeš and Varbanov [20] presented a further extension of the concepts of Total Sites [17] and Locally Integrated Energy Sectors [93]. They added the integration of renewable energy sources into the problem, emphasising the variability of both user demands and the renewables availability. Sustainability analysis has been a major consideration in the process synthesis. Sikdar [96] presented a framework for sustainability analysis to evaluate the data, leading one to a decision to accept, reject or re-work a solution.

Morrison et al. [97] presented an interesting application of solar thermal energy utilisation in food industry. They proposed to use captured solar heat in a way similar to heat pumping, thus upgrading waste heat flows to temperatures suitable for process use. The Pinch concept has been extended to renewable energy supply chain synthesis by Lam et al. [98,99,100] for assessing the feasible ways for transferring energy from renewable sources to customers in a given region. The studied region is partitioned into a number of clusters by using the developed Regional Energy Clustering (REC) algorithm. The energy planning and management is extended and illustrated in Regional Resource Management Composite Curve (RRMCC). It provides straightforward information of how to manage the surplus resources - biomass and land use in the region. Desai and Bandyopadhyay [101] proposed a scheme for efficient utilisation of lower-grade waste heat for power generation, using Organic Rankine Cycles. They provided a graphically assisted procedure for integrating an industrial process with an ORC thus efficiently reducing the process cooling demand and the need for external power import. Ghajar and Tang [102] presented the validity and limitations of the numerous two-phase non-boiling heat transfer correlations. The study presented a good opportunity for heat integration. It should be continued into advanced PI steps.

1.5.10. PRES'09

Gundersen, Berstad and Aspenlund [103] extended a previous work on Extended Pinch Analysis and design procedure (ExPAnD) where pressure and phase are considered together with the temperature. Bulatov, Perry and Klemeš [104] demonstrated an early stage energy technology tool EMINENT [105] on an application creating energy from the motion of waves. Harkin, Hoadley and Hooper [106] successfully applied process integration on carbon capture and sequestration cases. Lam, Varbanov and Klemeš [100,107] developed novel Regional Energy Clustering methodology based on Regional Resources Management Composite Curves. This can be used for minimising the CFP created by the biomass transportation. Al-Mutairi and El-Halwagi [108] developed a targeting tool for scheduling considerations in the retrofit of HENs. Polley, Picon-Nunez and Davados [109] used process integration methodology for the design of water and heat recovery networks for the simultaneous water and energy consumption. Important issues of e-learning and e-teaching of process integrations have been also presented by Sikos et al. [110].

1.6. Future trends – innovations in energy, resource and footprint targeting

Recent research has been expanding the scope of PI as well as the performance criteria for the system evaluation.

1.6.1. Energy planning using carbon footprint

Climate change has been growing in importance to the international community. Most of the attention has been focused on the carbon footprint (CFP) as a measure of the extent of greenhouse gas emissions impact. An interesting contribution by Foo et al. [88] deals with the "Carbon and Footprint-Constrained Energy Planning Using Cascade Analysis Technique". They presented algebraic targeting techniques for energy sector planning with CO_2 emission and land availability constraints. It is desirable to maximise the use of low carbon energy sources to reduce CO_2 emissions. This contribution provides an extension of the classic Pinch Analysis [7] for identifying the minimum amount of low- or zero-carbon energy sources needed to meet the national or regional energy demand, while not violating the CO_2 emission limits. Tan and Foo [111] and Tjan, Tan and Foo [112] extended the Pinch analysis to carbon emissions and energy Footprint problems. The water footprint problem had been examined by Klemeš, Lam and Foo [113]. A long needed contribution has been The Environmental performance Strategy Map based on the Life Cycle Analysis and quantifying the combined impact of various footprints — carbon, water, energy, emissions and the work environment footprints [114,115].

1.6.2. Extending total sites

An important innovation in the field of energy targeting and integration has been presented at PRES'07 by Perry et al. [93]. This was a result of collaboration between the UK and Hungary under several FP6 EC supported projects. The work presented an extension of the Total Site concept. Traditionally, Total Site meant only a set of industrial processes. This paper made another major step further by including commercial and residential energy users into the Total Site scope. The resultant process collections are termed Locally Integrated Energy Sectors. The method can be successfully applied to integrate renewables and consequently reduce the CFP of these locally integrated energy sectors. The attention to further development of the Total Site extension of Process Integration become during the recent period widespread [116,20]. Chew et al. [117] approached another very considerable task - the problem of the water site integration.

1.7. Some interesting case studies

A case study of pinch analysis was presented by Wising et al. [118]. They evaluated the potential for reducing the water and energy consumption by using pinch analysis approach. An existing pulp and paper mill was studied targeting the reduction of water consumption. A method for analysing energy, environmental, and economic efficiency for an integrated steel plant was presented by Larsson et al. [119]. Global mathematical models for steel making processes have been developed with the help of PI techniques. The traditional beet sugar manufacturing technology has a considerable detrimental impact on the environment. Vaccari et al., [120] gave an overview of the environmental problems in beet sugar processing. They applied Water Pinch and Thermal Pinch Analyses to assist in finding ways to drastically reduce both water and energy consumption. PI was applied to food industry. Kapustenko et al. [121] demonstrated the integration of a heat pump into the heat supply system of a cheese production plant in Ukraine. They analysed the opportunity of heat integration of an existing refrigeration unit into the process. A very interesting application of Heat Integration of evaporators with the remaining process has been presented by Axelsson et al. [122]. Their observation was that significant energy savings can be made in the pulp and paper industry by implementing process integrated evaporation (termed “PIvap”). Using pinch tools they found a solution where 1.3 GJ/ADt (GJ per Air Dried t) of pinch violations were solved and 1.1 GJ/ADt of excess heat saved. Pulp-and-paper Kraft mills feature significant energy demands. Savulescu and Alva-Argáez [123] have proposed a PI methodology to systematically address direct heat transfer (DHT) aspects in the Kraft mill energy system retrofit context. Their observation shows that energy-efficient non-isothermal mixing points should be located at the end of a stream. From the process perspective, mixing should be below pinch or above to eliminate the inefficiencies, due to DHT cross-pinch. Additionally, mixers located away from the pinch represent degrees of freedom to design an optimal heat transfer network. Levasseur et al. [124] have presented an application of classical heat integration techniques with process changes to liquor evaporation in pulp-and-paper mill. The system involves multi-effect evaporation. The considered modifications were reduction of ΔT_{min}, as well as variation of the pressures of evaporation effects. As a result, energy savings of up to 20% were reported. Accounting for the non-continuous operation of pulp-and-paper mills, Morrison et al. [125] presented a case study for varying paper grades. They applied the Time Slice Model for batch heat integration. A powerful tool, Site-Model, was introduced by Hirata et al. [126]. To handle the trade-off between the flexibility and the interactions, all units should be managed simultaneously. The tool implements a large-scale MILP model for the utility system optimisation. Nordgren et al. [127] presented heat balancing study of a metallurgical process with the aim to perform a subsequent Heat Integration project. The paper is a part of a project which aim is to develop a PI model for the Swedish iron ore company LKAB’s production system in Malmberget. The authors analyse the various processing zones of the furnaces and the opportunities for heat recovery using external heat exchangers. Matsuda et al. [128] applied heat integration total site technology to a large industrial area in Japan to further improve performance of their already highly efficient process plants. Tovazhnyansky et al. [129] successfully completed process integration based synthesis of sodium hypophosphite production. Promvitak et al. [130] applied the heat integration methodology on the crude distillation unit. Varbanov and Friedler [131] boosted the energy convertion efficiency of fuel cell. Parisutkul et al. [132] improved the energy efficiency of the natural gas separation plant. Atkins et al. [133] completed carbon emission pinch analysis of New Zealand Electricity sector and Markowski et al. [134] fermentation based hydrogen plant connected with sugar factory. Varga et al. [135] by using heat integration improved energy efficiency of several units in MOL refineries in Hungary and Slovakia. Pavlas et al. [136] implemented the heat integrated heat pumping for biomass gasification processing.

2. Optimisation for energy savings and reduced emissions

The field is enormously wide. Therefore, this short overview is targeting optimisation methodologies which have the strongest impact on energy saving and pollution reduction.

2.1. Integrated synthesis of process and HENs

Nagy et al. [137] developed a new algorithmic method for the integrated synthesis of processes and HENs. Different methods exist for algorithmic process network synthesis (PNS) as well as for heat exchanger-network synthesis, but they cannot easily be integrated. For instance, the flow rates of streams are not specified a priori in PNS; in contrast, the flow rates and temperatures of hot and cold streams have to be known as inputs in HEN synthesis (HENS). This difference can be attributed to the fact that the former is macroscopic in nature, while the latter is mesoscopic in nature, giving rise to the characteristic differences between them. Both PNS and HENS inevitably encounter combinatorial complexity, which is magnified profoundly when they are integrated, due to their interactions. The P-graph framework developed earlier for PNS [138] has been extended to the integrated synthesis of process and heat exchanger networks. This new method resorts mainly to hP-graphs adapted from the P-graphs in conjunction with the appropriate selection of inherent intervals of temperature range. Therefore, it focuses on the establishment of an appropriate technique for the integration of PNS and HENS [137]. The resultant technique is largely based on combinatorial algorithms. The efficacy of the proposed approach was illustrated by the solution of an industrial problem.

2.2. Scheduling in heat integration and water reuse for batch processes

Foo et al. [73] present a two-stage procedure for the synthesis of a maximum water recovery network for a batch process system, covering both mass transfer-based and non-mass transfer-based water-using processes. Adonyi et al. [139] developed a new algorithmic method for heat integration of batch processes. By nature, batch process scheduling and heat integration are two significantly different highly complex optimisation problems. Many algorithmic and heuristic based methods exist for solving heat integration problems by resorting to pinch technology; superstructure based mixed integer programming, and integration with process network synthesis. These methods have been developed for continuous processes where scheduling is of no concern. These two different problems can be solved sequentially, i.e., solving scheduling first and then heat integration or vice versa. Since the solution of one of them influences the other, the result of this simplistic approach is usually very poor. An integrated consideration of scheduling and heat integration may provide appropriate solution. Since no method known up to that time for solving the integrated model, the development of a new method was desired for effective design and operation of batch processes. The main issue was how to operate tasks with potential heat exchange simultaneously without sacrificing the quality of the scheduling solution. The proposed procedure is based on the branch-and-bound framework, where two optimisation problems, the scheduling and the heat integration one, are considered simultaneously instead of consecutively.

2.3. Batch scheduling with minimising cleaning costs

The cleaning for batch processes, especially, paint production systems have been examined by Adonyi et al. [140]. Due to the large variety of options offered to customers, batch production schemes are widely used in paint industry implying that scheduling plays an important role in optimal allocation of plant resources among multiple products. Since in a batch process, the cleaning of equipment units is the major source of waste, waste minimisation is also to be taken into account in determining the schedule. In the paint production, a product is produced by four successive tasks: grinding, mixing, storing the intermediate materials, and packing. Grinding, mixing and storing are batch type operations while packing is continuous. A task cannot be performed by a dedicated equipment unit, because there are usually more tasks than equipment units. An equipment unit is assigned to each task for a time interval where the length of the interval must not be shorter than the processing time of the related task. Changeover time is defined for an equipment unit if cleaning is necessary. The whole amount of the intermediate material is used by the successive tasks. Traditionally, such assignment of equipment units to tasks and schedule of tasks is generated that have minimal makespan. This schedule provides the highest efficiency of the production system with the possibility of unnecessarily large waste generation. For determining the schedule of tasks that requires minimal cleaning cost, the objective function of the problem has to be modified. While in the original problem the makespan, in the reformulated problem the cleaning cost must be minimized. This reformulation has minor effect on the solution procedure. Therefore, an effective solver for the original problem is useful for the reformulated problem also. The formerly developed S-graph framework [141] proved to be highly effective in solving multipurpose batch scheduling; it has been specialised by Adonyi et al. [140] for solving paint production scheduling problems including waste minimisation. The efficacy of the new approach is illustrated with the solution of large-scale paint production scheduling problems.

2.4. Strategic roadmap - decomposition versus integration for process optimisation

The decomposition principle in process design has been used by researchers since the 1970's — e.g. [142]. Friedler and Fan [143] drafted a strategic roadmap for the development of process optimisation, analysing the interactions between the decomposition and integration principles. They have identified a number of threats to the optimality and feasibility of the process designs when applying decomposition and suggested measures to counteract the problems, centred on the concept of the integration of the methodologies for the component design problems. This concept has revealed the need for algorithmic generation of the component models and the necessary interfaces enabling the interactions of the models and methods. The algorithmic generation of the models allows mainly ensuring their validity and completeness of the network superstructures. One efficient way for algorithmic model generation has been using P-graph [138,144,145].

2.5. Looking inside the processes — process intensification

Reay [146] has presented the role of PI and intensification in cutting greenhouse gas emissions. He identified the challenges that intensification is able to meet across a range of sectors of industry and commerce as they relate to greenhouse gas control. He mentioned that the possibility of increased local production and the growing use of biological renewable feedstock open up new challenges and opportunities for those active in integration as well as intensification. He stated that between 1900 and 1955 the average rate of global energy use rose from about 1 TW to 2 TW. Between 1955 and 1999 energy use rose from 2 TW to about 12 TW. To 2006, a further 16% growth in primary energy use was recorded world-wide. The conclusions are that process intensification, although yet to fully emerge as an established technology in the process industries, offers significant opportunities for carbon reductions in sectors ranging from chemicals to food and glass manufacture.

2.6. Contributions from PRES conferences

Heat integration of chemical multipurpose batch plants was studied by Sanmarti et al. [147]. It was based on directed graphs and exploiting the optimisation power of combinatorics. This approach has been further developed by Sanmarti et al. [148] into S-graphs. Scheduling problems have been solved also for batch water networks. One example is the work by Chen et al. [149], who have developed a method for synthesising water-using networks with central reusable storage for batch processes. A further development has been presented at PRES'09 [150] on property-based water-using networks in batch processes. The wide spectrum of the batch applications can be illustrated by the work performed by an international team on profitability analysis of batch reactive distillation [151].

The problem of HENs flexibility and operability had been dealt with by Tantimuratha et al. [152]. They proposed simple MILP models to solve the problem. However, a closer combination with pinch analysis had yet to come. Nagy et al. [153,137] presented an algorithmic approach for integrated synthesis of process and HENs. This work focused on the establishment of an appropriate technique for the integration of PNS and HENS. The resultant technique was largely based on combinatorics and combinatorial algorithms. This novel approach opened a new opportunity of the PI approach. Halasz et al. [154,155] presented a novel tool, especially important for the retrofit design. An optimal design and operation of an existing steam-supply system of a chemical complex was demonstrated using P-graph, the decision-mapping, combinatorial algorithms, and the accelerated branch-and-bound method. Adonyi et al. [139] introduced a novel S-graph approach to incorporate heat integration in batch process scheduling. The proposed procedure is based on the branch-and-bound framework, solving the scheduling and the heat integration problems simultaneously instead of consecutively. Varbanov et al. [156] proposed a method to synthesise industrial utility systems capable of cost-effective decarbonisation. It is based on improved models of utility equipment components and on an improved model and procedure for optimal synthesis. The environmental impact of utility systems was integrated into a synthesis model, which is dictated by the need for significant reduction of CO_2 emissions.

Application of pinch technology was presented by Ravagnani et al. [157] to synthesise a HEN and further employing a genetic algorithm. Synthesis of HEN by using mathematical model approach was presented by Markowski et al. [158,159]. Heat exchanger cleaning is postulated to maximise the avoided loss understood as the value of energy recovered if cleaning the HEN, minus the value of energy recovered without HEN cleaning, minus the cost of HEN cleaning. The mathematical formulation of the avoided loss is given and the computational approach to its maximisation is outlined. Ullmer et al. [160] presented a methodology and software for the synthesis of process water systems. They developed an integrated strategy for the design of industrial process water systems to determine the optimal cost network, taking into consideration multiple contaminants and various possibilities of water reuse and regeneration. The efficiency and applicability of software was demonstrated on a process water system of an oil refinery. Hugo et al. [161] presented a multi-objective optimisation model for strategic hydrogen infrastructure planning. The optimisation is conducted in terms of both investment and environmental criteria, with the ultimate outcome being a set of optimal trade-off solutions representing conflicting infrastructure pathways. This model has considerable potential, especially into the regional energy integration.

Ponton [162] shared the experience on using web based distance learning for continuing professional development in the control, modelling, and optimisation courses. Transformation of process data into a meaningful description is very important to process integration. Drahoš and Ružička [163] studied the characterization of process data such as pressure, temperature, and concentration by using time series analysis. Pistikopoulos [164] gave an overview of the mathematical foundations of multi-parametric programming for different models. He also presented the application of model-based optimal control with emphasis on designing off-line affordable advanced parametric controllers for chemical processes.

Friedler and Varbanov [165] presented an application of the CHP concept in combination with the P-graph framework for designing complex systems for energy supply and conversion. Two kinds of High-Temperature Fuel Cells (HTFC) were considered — Molten Carbonate Fuel Cells (MCFC) and Solid Oxide Fuel Cells (SOFC). The paper presents a tool for the evaluation of energy conversion systems involving Fuel Cell Combined Cycles (FCCC) subsystems, utilizing biomass and/or fossil fuels. This task involves significant combinatorial complexity, efficiently handled by the P-graph algorithms, producing cost-optimal FCCC configurations. It also accounts for the carbon footprint of the various technology and fuel options. The results show that such systems employing renewable fuels can be economically viable for a wide range of economic conditions, mainly due to the high energy efficiency of the FC-based systems, having the potential to reduce the carbon footprint of energy supply by 50–75%.

Tan [166] presented an accelerated modification of the popular Simulated Annealing optimisation algorithm employing swarm intelligence techniques. Two modified SA algorithms have been developed by incorporating parallel searching and information sharing features found in swarm-based techniques such as PSO and SFLA, as well as an adaptive cooling schedule. Tests on three chemical process network design and synthesis problems showed that the modifications yield improvements in search characteristics as compared to conventional SA and other optimisation algorithms. The new algorithms needed fewer function evaluations to reach the final solution and gave more robust and consistent results when tested repeatedly for the same problem. An approach to multi-period HEN synthesis using Simulated Annealing [167] has been suggested. It uses a completely evolutional strategy starting from a trivial network topology connecting all hot streams to coolers and all cold streams to heaters. They stated that the performance of the optimisation procedure is comparable to the existing Mathematical Programming based ones. The method does not rely on any superstructure, is not subject to decomposition of the main problem, and can explore a greater search area, increasing the probability of obtaining the global optimum. Sikos and Klemeš [168,169] successfully optimised reliability, availability and maintenance of heat exchanger networks and contribution to efficient waste minimisation and management. Kim [170] performed a conceptual optimal design applying a process simulator. Touš et al. [171] presented an alternative solution and optimisation to an integrated system of biomass and/or alternative fuel integrated into a complex energy producing system. Meszaros and Čirka [172] performed a control analysis with inner recycle of hybrid separation process. Friedler et al. [173] developed a methodology for optimising the HEN design for Multi-Operation Using P-Graph.

3. Conclusions and future outlook

Modern societies must face numerous issues in seeking to secure a sustainable energy supply, reduce climate changes, and ensure food production. The rapid increase in global energy consumption makes the problem more complicated. Recent oil and gas crises have shown the vulnerability of the societies in terms of climate changes and energy supplies. However, due to the complexity of the global challenges, it can be realised that each person or team has limits to the issues that they could effectively address. This is the reason why this overview is based upon the specialised inputs from a number of skilled scientists and technologists. Taken as a whole, the reviewed papers address many of the challenges pertaining to global climate change and to the impacts of the decisions that can be made.

New insights are emerging on energy-related problems. Many of them seem to be rather straightforward, however most of them have not yet been satisfactorily solved. Many of the problems have been addressed annually at the PRES conferences held during the last 13 years. Some of them were summarised by Dovì et al. [174]:

(i) Diversification of energy sources and supply chains; regional energy sustainability zones and inter-zone integration.
(ii) The mass storage of energy — especially of electricity and heat.
(iii) The energy efficiency and energy saving attitude being accepted as a priority by society.
(iv) The change of the societal approach away from wasting energy.
(v) Sustainable energy solutions for transport — technology, management and societal acceptance.
(vi) Sustainable energy solutions for developing countries.
(vii) Sustainable energy for securing fresh water for the world's growing human population.

However they have been still many other issues which should be further explored in the future as the new avenues in sustainable energy generation supported by efficient energy carriers. The list could be considerably extended. It is a positive sign that some of the big players are researching these issues see e.g. [175]. However, much more collaboratively orchestrated work is needed to find proper answers to these challenges. The PRES series of conferences has been designed to provide the necessary forum and networking opportunities for accelerating the scientific and engineering progress in the field.

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