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PROCESS INTEGRATION FOR INDIVIDUAL PROCESSES, INDUSTRIAL SITES, AND MACRO ENERGY SYSTEMS

INTEGRACE PROCESŮ PRO INDIVIDUÁLNÍ PROCESY, PRŮMYSLOVÉ ZÓNY A MAKRO ENERGETICKÉ SYSTÉMY

SHORT VERSION OF HABILITATION THESIS

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ABOUT THE AUTHOR

Dr Timothy G. Walmsley was born and raised in Hamilton, New Zealand. After completing high school, he began a Bachelor of Engineering in Materials and Process Engineering at the University of Waikato, Hamilton. In 2010, he completed his B.E. degree and soon after embarked on pursuing a PhD in Process Engineering also at the University of Waikato, which was completed in 2014. His thesis entitled "Heat Integrated Milk Powder Production" combined with subsequent post-doctoral research in the Waikato Energy Research Group established a specific energy performance level for milk powder production. In 2015, Dr Walmsley was elected a Member of the Institute of Chemical Engineers (MIChemE), UK, and award the status of Chartered Chemical Engineer (CEng) of the UK Engineering Council. In 2016, IChemE awarded Dr Walmsley the International Young Chemical Engineer in Research Award. He

currently serves as International Editorial Board Member for the Journal of Cleaner Production (Elsevier) and Co-Chair of the International PRES Conference series (conferencepres.com). He joined the Sustainable Process Integration Laboratory - SPIL, led by Professor Jiří J. Klemeš, within the Faculty of Mechanical Engineering, Brno University of Technology in 2017 as a founding member of the team.

The main theme of his research has centred on designing sustainable systems – unit operations, processes, industrial sites, regions and global – by applying novel process modelling, integration, and optimisation methods. Dr Walmsley has published 27 articles in international journals with Impact Factors and an additional 40 further articles with DOI.

1 INTRODUCTION

1.1 BACKGROUND

Process Integration

In the 1970's, the world oil crisis drove innovation in the industrial sector resulting in vast improvements in thermal energy efficiency for many large energy users in chemical processing. The oil crisis gave life and purpose to the research area of Process Integration (PI). The PI concept embodies a holistic approach to process design that emphasises the system-wide performance over individual sub-system efficiency. Under the PI paradigm, individual sub-systems are engineered from the outset to fit together in such a way that is advantageous to the whole. The PI methodology addresses the design of both new systems as well as the retrofit and revamp of existing processes.

PI plays a key role in addressing energy and resource efficiency and sustainability improvement in the process industries as well as macro energy systems [1]. There are three approaches to PI [2]: (1) graphical methods including Pinch Analysis (PA) that are based on thermodynamics, (2) Mathematical Programming (MP) methods, and (3) hybrid approaches. Application of PI techniques to a wide variety of industries and multiple scales have helped realise meaningful increases in system performances for individual processes, Total Sites, and macro energy systems [3].

Total Site Integration

Total Site Heat Integration (TSHI) was initially introduced by Dhole and Linnhoff [4]. TSHI is a strategy for the integration of large multi-process sites to improve site-wide energy efficiency that has focused on exploiting the steam utility system to recover and place heat [5]. The method prioritises integration of individual processes and zones (i.e. defined areas of integrity [6]), before integrating across an entire site using the utility system [7]. Total Site (TS) source and sink profiles are composites of shifted Grand Composite Curves (GCC) from individual processes and applied to calculate TS targets for heat recovery, utility use, and shaft work/power generation [8]. Shortly after its initial development, Klemeš et al. [5] summarised successful applications of TSHI to an acrylic polymer manufacturing plant, several oil refineries and a tissue paper mill, which all showed utility savings between $20 - 30$ %. The PhD thesis of Raissi [9] presents much of the early developments of TSHI.

Energy Systems Planning

PI also applies to macro energy system planning. Carbon Emissions Pinch Analysis (CEPA) was first developed by Tan and Foo [10] and is based on the application of traditional PA techniques to broader macro-scale applications such as regional and national electricity generation sectors [11]. Sectorial and regional studies have been conducted for power systems emissions constraint planning with CCS $[12]$ and for multi-period scenarios $[13]$ and variable CO₂ sources and $CO₂$ sinks [14]. In the New Zealand context, CEPA has been applied to the national electricity sector [15] to show how increased electricity demand in 2050 can be met and the generation mix optimised for minimum energy cost [16]. Energy costs were based on the Pinch Analysis of Energy Return on Investment (EROI).

EROI was proposed by Hall et al. [17] and continues to be the subject of ongoing research in recent literature [18]. Conceptually, EROI is simple. It compares the amount of useful energy derived compared to the amount of energy expended to process, generate, and distribute the useful energy. As a common example, crude oil extraction with an EROI of, say, 100, would represent that the energy equivalent of 1 barrel of oil, in various forms such as embedded energy and electricity to drive pump shafts, is required to extract 100 barrels of crude oil. The EROI concept has found a wide variety of applications [19]. EROI, as a metric representing an energy resource,

has been linked to the quality of life [20]. Weißbach et al. [21] suggested the minimum acceptable EROI is 7, below which there is an insufficient return to justify action. It has been applied to try to explain the decline in oil production from the viewpoint that as conventional oil runs out, unconventional oil reserves will be more energy intensive to access, which will result in lower financial returns of investments [22]. Similarly, a correlation between oil prices and EROI over time has been attempted [23]. These applications highlight the benefits of knowing and understanding the EROI for different natural resources.

Minimising GHG footprint through CEPA and maximising the EROI are often competing objectives. Effective production of energy with high EROI values is crucial to economic growth, industrial manufacturing, employment and the general economic well-being of citizens [24]. CEPA, on the other hand, quantifies the environmental impact in terms of emissions of using energy. CEPA is a graphical method for showing how much carbon emissions are contributed from each part of an energy sector (e.g. electricity, transport) and exploring possible pathways for modifying the energy system to meet fixed emissions targets.

1.2 THESIS STRUCTURE

Chapter 2 presents an overview of the research fields of interest. In Chapters 3, 4, and 5, the contributions to literature are divided by the scale of application. Within each of these chapters, the research contributions are divided into (1) Novel and Innovation Methods and (2) Case Studies. Chapter 3 encompasses research that addresses the PI of individual unit operations. The major line of work focused on milk powder production energy efficiency with the creation of novel methodology being an offshoot of detailed case studies. Chapter 4 elevates the PI focus to the Total Site level. Several contributions have been made in this area with the most significant being the application of novel Total Site methods for low-temperature sites that use hot water as a standard utility. Chapter 5 showcases contributions that deal with macro energy systems integration and planning. The contributions in Chapter 5 centre around the extension and application of Pinch Analysis and Energy Ratio analysis to sustainable energy planning with a focus on the New Zealand energy sectors of electricity, transport and process heat.

2 RESEARCH FIELDS OF INTEREST

2.1 OVERVIEW

Process Integration (PI) is the systematic process and art of engineering process, utility, regional, and national systems as a single entity that respects practical constraints to reach maximum levels of energy and resource conversation. [Figure 1](#page-7-3) illustrates this point using puzzle pieces. With the appropriate design of process systems to optimally fit together with the utility and energy supply systems including renewable energy, the performance of the entire system can be raised. The principles of PI apply from the process level through to the national and global energy system levels. To maximise benefits, design decisions at every level need to be considered and optimised within the context of the greater whole.

Figure 1: The integration of process, utility and energy supply systems for maximum overall performance.

The research presented in this thesis focused on applying novel and innovate process analysis, modelling, integration, and optimisation techniques for the integrated design of sustainable process and energy systems. The scales of application include individual unit operations, Total Sites, and regional and national energy sectors. The research is the result of on-going collaborations with researchers from the University of Waikato (New Zealand), Universiti Teknologi Malaysia (Malaysia), University of Kassel (Germany), and Technische Hochschule Ingolstadt (Germany). The bulk of the research was undertaken at the University of Waikato, New Zealand before taking up his present appointment at Brno University of Technology as a researcher in the Sustainable Process Integration Laboratory – SPIL team.

2.2 PROCESS INTEGRATION AND OPTIMISATION OF UNIT OPERATIONS

At the process level, novel methods include: (1) a derivative approach for determining the costoptimal area allocation within a Heat Exchanger Networks; (2) Heat Exchanger Network retrofit methods including graphical and tabular tools as well as automation for scalability; (3) improved numerical and graphical procedures to meaningfully determine targets for exergy requirement, rejection, and loss. These methods have been applied to several case studies to realise radical stepimprovement opportunities in energy efficiency. The main case studies include (1) the integration and optimisation of milk evaporation system through the appropriate placement of vapour recompression, (2) the integration of milk spray dryers through conventional heat recovery and novel heat pump designs, and (3) experimental and numerical analysis of milk powder fouling $-$ a key barrier that prevents full realisation of milk spray dryer energy recovery.

2.3 TOTAL SITE INTEGRATION

At the Total Site level, the research interests focused on advancing the application of TSHI concepts to low-temperature processing sites such as dairy, meat, and pulp and paper factories. The research has developed several novel methods including (1) TSHI concepts for waste heat recovery through the application of heat pumps, absorption chillers, and assisted integration, (2) an integrated design method for multi-effect evaporation systems with vapour recompression operations, (3) the Unified TSHI method for targeting, optimising and designing Heat Exchanger Networks for sites that use non-isothermal utility, and (4) an extend TS method covering mass, heat and power integration through the combination of TSHI and P-graph. The case studies in this area cover (1) TSHI of single and multi-plant dairy factories, (2) Heat Recovery Loops for sitewide dairy factory heat integration, and (3) Total Site utility systems design using P-graph with consideration for an electricity spot-price and environmental impacts such as GHG emissions, particulates (P_{10}) and water use.

2.4 MACRO ENERGY PLANNING AND INTEGRATION

At the macro-level, several methods for energy planning, linking Carbon Emissions Pinch Analysis with Energy Return on Investment, as well as advancing the understanding and application of Energy Ratios as energy planning metrics have been developed. In addition, a Pgraph based targeting method for municipal waste-to-energy networks has recently been formulated. A series of case studies in this area focused on the New Zealand energy sectors with comprehensive analysis and energy planning for the electricity, transport and process heat sectors. An additional case study on the wind energy potential for electricity generation in New Zealand was also undertaken.

3 PROCESS INTEGRATION AND OPTIMISATION OF UNIT OPERATIONS

3.1 NOVEL AND INNOVATIVE METHODS

The reported novel and innovative methods for the integration, optimisation, and retrofit of unit operations centre on three areas: greenfield HEN design using the new Cost Derivative Method [\(3.1.1\)](#page-9-2), a new and automated HEN retrofit method [\(3.1.2\)](#page-9-3), and a new method of determination of process exergy targets [\(3.1.3\)](#page-9-4).

3.1.1 The Cost Derivative Method (CDM) for New Heat Exchanger Networks

This contribution [25] presented a novel Cost Derivative Method for finding the optimal area allocation for a fixed Heat Exchanger Network topology to achieve minimum total cost. The concept of the novel approach was to incrementally add, remove and shift the heat transfer area to exchangers where the greatest economic benefits are returned. To allow the use of derivatives, the method focused on the variable cost component for heat exchangers with the assumption that fixed costs are a constant for a given HEN. This meant the cost function with respect to the area of the heat exchanger in a network became continuous and possible to solve using derivatives.

3.1.2 New Heat Exchanger Network Retrofit Method based on Bridge Analysis

Graphical and diagrammatical tools elevate the level of insight for the engineer into the thermodynamic and practical limitations to Process Heat Integration and HEN retrofit. As a result, problems may be decomposed into more understandable problems. In addition, retrofit tools also provide an effective platform to communicate engineered solutions to industrial companies. However, a severe limitation of these tools is poor scalability. Large-scale HENs present a challenge as insights gained at a small-scale are more obscure for large HENs. A degree of automation of insight-based retrofit procedures including heuristics is needed to help extend its application of large-scale HENs and to minimise human error during the analysis procedure.

In this area, the contribution has been two-fold. First, an attempt has been made to improve the graphical representation of the HEN retrofit problem [26] while also providing the numerical alternative [27] that has developed into the Automated Retrofit Targeting (ART) algorithm [28]. To demonstrate the new method and tool, a refinery case study with 27 streams and 46 existing heat exchangers demonstrated the retrofit method's potential. For the case study, the Automated Retrofit Targeting algorithm found 68,903 feasible unique retrofit opportunities with a minimum 400 kW/unit threshold. The most promising retrofit project required 3 new heat exchanger units to achieve a heat savings of 4.24 MW with a favourable annualised profit and a reasonable payback period.

3.1.3 New Exergy Pinch Analysis Method for Sub-Ambient Processes

Sub-ambient processes such as a refrigeration system are a highly energy intensive area in chemical industries. Refrigeration systems require a high level of process cooling using a combination of compression and expansion operations. It is crucial to optimise heat transfer between the utility system and the process streams including the placement of compression and expansion operations to minimise the exergy losses and work as much as possible. Exergy Analysis is defined as a systematic tool to determine exergy content in the processes so that compressor shaft work can be analysed.

Through a collaboration with Universiti Teknologi Malaysia, a series of work was undertaken to improve the basis for setting exergy targets with the contribution being captured by [29]. In this capstone publication, new tools such as a set of Exergy Problem Tables and Exergetic Grand Composites are introduced. One of the fundamental differences between [29] and the approach of Marmolejo-Correa and Gundersen [30] was an assumption of horizontal heat transfer, which matches the conventional formulation of the Grand Composite Curve. A graphical example of the new Exergetic Grand Composite is presented in [Figure 2.](#page-10-1) Application of this tool helped to determine exergy targets for rejection, requirement and avoidable losses.

Figure 2: Exergy Grand Composite Curve (Ex-GCC) of the refrigeration system with minimum approach temperature of 10 ºC.

3.2 CASE STUDIES

The majority of case study research on unit operations have centred on the production of milk powder from milk. Minimising the energy demands and overcoming barriers to implementation of energy efficiency projects are the focuses of the present section.

3.2.1 Unit Operation Energy Integration and Optimisation in Milk Evaporation Systems

Thermal and mechanical vapour recompression technologies find excellent application in a wide range of evaporation and distillation systems. In milk evaporation systems, vapour recompression units directly compress vapour flows drawn from the product on the tube-side ("evaporator") to a higher pressure and temperature for use as the condensing vapour on the shellside ("condenser"). As a result, this arrangement creates a so-called open cycle heat pump. The analogy between vapour recompression and conventional heat pumps also extends to the idea of appropriate placement in Pinch Analysis, which states that a heat pump should upgrade heat from below the Pinch for use above the Pinch [31]. Purposeful design and integration of the evaporation system to complement the heat demands of neighbouring processes provide greater opportunities for energy and emissions savings.

This series of contributions to literature, represented by [32], focused on applying Pinch Analysis to an industrial milk evaporator case study to quantify the potential energy savings by implementing the appropriate placements of vapour recompression technologies. A detailed heat and mass balance process model of a multi-effect falling film milk evaporator system, including

both MVR and/or TVR options, was implemented in an Excel^{TM} spreadsheet. The model was validated for a current industrial set-up using plant data. The Grand Composite Curve played a critical role in identifying areas for process modifications and placement of vapour recompression that results in energy reduction. After the development of a design concept, it was replicated in the Excel model to derive a new set of stream data. With several iterations between modelling and Pinch Analysis, a new final design required 78 % less steam (6,397 kW) at the expense of 16 % $(364 \text{ kW}_{\text{ele}})$ more electricity use. The estimated cost savings associated with the improved design was 942,600 NZD/y (\sim 14,200,000 CZK) and the emissions reduction was 3,416 t CO₂-e/y.

Figure 3: Development of an evaporation system design using the Grand Composite Curve, given Effects 1 and 2 are both integrated with MVR. (A) Identification of potential energy savings. (B) Final GCC for new MVR/MVR evaporation system design.

3.2.2 Integration and Optimisation of Milk Spray Dryers

Spray dryer exhaust heat recovery can typically increase dryer energy efficiency by $10 - 20$ % [33], but it is complicated by the low heat transfer coefficient of air and the presence of powder particulates that may foul the heat exchanger surfaces. Increasing energy efficiency in milk spray drying is an important topic for New Zealand because the results of the New Zealand dairy industry heavily impacts the national economy. The installed capacity of milk spray drying in New Zealand reached an estimate of 300 t/h in 2013 with a consumption of around 29 PJ/y of thermal energy. Milk powders supply about 20 % of New Zealand's exports.

This contribution [34] to the literature reported a thermo-economic design optimisation of an industrial milk spray dryer liquid coupled loop exhaust heat recovery system. Incorporated into the analysis is the ability to predict the level of milk powder fouling over time and its impacts on heat transfer and pressure drop. The numerical predictions were based on the model from [35], which was formulated from experimental fouling tests. For the dryer exhaust heat exchangers, the compact heat exchanger design applied finned round tube, bare round tube and bare elliptical tube. Modelling results showed that spray exhaust heat recovery is economically viable for the considered industrial case study. The best liquid coupled loop heat exchange system required a finned tube heat exchanger to recover heat from the exhaust air with a face velocity of 4 m/s and 14 tube rows, which gives a net present value of 2,900,000 NZD (43,500,000 CZK) and an internal rate of return of 71 %.

3.2.3 Fouling on Milk Dryer Exhaust Heat Transfer Surfaces

A significant challenge associated with the recovery of waste heat from milk dryer exhaust gases is, the air contains a small amount of powder that may deposit on the face and surfaces of a heat exchanger. The following three articles presented experimental and numerical research targeted at addressing this specific challenge. The purpose of this series of experimental and numerical work was to comprehensively quantify the issue of heat exchanger fouling for milk spray dryer exhaust heat exchangers.

Predicting the deposition during the production of milk powder was identified as a possible avenue for creating new designs and selecting processing conditions that minimise particle deposition for dryer exhaust heat exchangers. Numerous studies had looked at characterising various aspects of milk powder deposition, agglomeration and caking. However, the literature lacked a fundamental and validated criterion that describes the deposition of milk powder particle impacts with short contact times $(<1$ s).

In this first contribution [35] focused on milk powder deposition, standard solutions to the contact mechanics problem of a spherical elastic particle with an adhesive surface impacting a rigid plate at normal and oblique angles formed the basis to derive a semi-empirical criterion that described whether a particle sticks after impacting a wall. To validate the criterion, the determining factors of skim milk powder deposition, which are air temperature, water activity (i.e. relative humidity), plate (or wall) temperature, and particle size, velocity and impact angle, were isolated and experimentally tested using an impingement jet test. [Figure 4](#page-12-0) shows the collation of experimental test as applied to validate the semi-empirical model.

Figure 4: Combined effect of particle size, impact angle and velocity on deposition.

A second paper in the area [36] reported fouling and pressure drop analysis of milk powder deposition on the front of parallel fins. The work introduced a novel lab-based test that simulated powder deposition on a bank of parallel plate fins at spray dryer exhaust air conditions. The fin bank acted like the face of a typical finned tube row in an exhaust recuperator.

The aim of this study was to look at how deposition on the front of fins may be affected by the air conditions. Results showed similar characteristics to other milk powder deposition studies that exhibit a dramatic rate increase once critical stickiness levels are reached. As powder deposited on the face of the fins, the pressure drop across the bank increased until an asymptote occurs, indicating that the rates of deposition and removal had become similar. For very sticky conditions, deposition on the face of the fins caused a rise in the pressure drop by 65 %. The pressure drop was successfully related to the percentage of the open frontal area of the fins with and without deposition.

The final paper [37] in this area aimed to characterize the deposition of skim milk powder on a single bare tube in cross-flow, as shown in [Figure 5.](#page-13-0)

(a) Front and side views of deposition on a circular tube.

(b) Front and side views of deposition on an elliptical tube.

Figure 5: A comparison between fouling on (a) a circular tube compared to (b) an elliptical tube.

4 TOTAL SITE INTEGRATION

4.1 NOVEL AND INNOVATIVE METHODS

Between 20 % and 50 % of world energy consumption is lost as waste heat through energy conversion and transportation in manufacturing processes. Within industrial Total Sites and Locally Integrated Energy Systems, there is much opportunity to recover, upgrade and re-integrate heat that is currently rejected. The following articles focused on developing novel methods to improve TSHI couple with a demonstration through appropriate case studies.

4.1.1 Total Site Heat Integration Concepts for Waste Heat Recovery

This first line of research centred on the recovery of wasted heat, i.e. heat below the Pinch that is normally rejected to the environment. The first contribution [38] was a collaborative effort with the Universiti Teknologi Malaysia and Pázmány Péter Catholic University. This contribution presented a new Total Site Heat Integration concept that integrates heat, power, and cooling. The waste heat technology considered for cooling generation were Absorption Chiller and Electric Compression Chiller as shown in [Figure 6.](#page-14-2)

Figure 6: A Total Site with an integrated centralised cooling system.

The second contribution to this area [39] introduced an effective Total Site targeting methodology to integrate open cycle heat pump systems, i.e. vapour compression technologies, into an integrated industrial energy system for enhancing overall site energy efficiency. Vapour compression systems upgrade low-grade waste heat by supplying a low quantity of high-pressure steam or mechanical work (mechanical-compressor) to generate higher pressure steam, as is common with evaporation systems.

Industrial waste heat and high-quality steam demand were simultaneously reduced through open cycle heat pump integration. The energy reduction and cost-benefit of thermo-compressor and mechanical-compressor installations were compared through a literature case study. The case study showed a deficit of heat at the Medium-Pressure Steam level and a surplus of heat the Low-Pressure Steam level, which was identified as a candidate for compression according to the appropriate placement principle for heat pumps. For the case study, a four-stage mechanical vapour compression system and two-stage thermal vapour compression system resulted in energy cost reductions of 343,900 USD/y (\sim 7,086,000 CZK/y) and 168,829 USD/y (\sim 3,479,000 CZK/y).

A final contribution in this area [40] presented a new method for calculating assisted heat transfer and shaft work targets for an example TS problem. Analysis results showed that assisted heat transfer increases TSHI only when a process heat recovery pocket spans the Total Site Pinch Region. The maximum assisted TSHI can be targeted by comparing each heat recovery pocket to the Site Utility Grand Composite Curve using background/foreground analysis as illustrated in [Figure 7.](#page-15-0)

Figure 7: (A) New Total Site Profiles including assisting segments of pockets from Process A and D compared to the conventional method. (B) Targets for assisted heat transfer and shaft work using the Site Utility Grand Composite Curve and the Grand Composite Curve pockets from Process A, B, and D.

Where heat recovery pockets span two steam pressure levels away from the TS Pinch Region (usually above), the example showed the potential for assisted shaft work production. In this case, the source segment of the heat recovery pocket generates steam (e.g. MPS), which replaces steam that would otherwise have been extracted from a steam turbine. The sink segment of the heat recovery pocket consumes lower pressure steam (e.g. LPS), which is extracted from the turbine. If a heat recovery pocket falls outside these two situations, the entire pocket should be recovered internally to a process.

4.1.2 A Total Site Heat Integration Design Method for Integrated Evaporation Systems Including Vapour Recompression

Evaporation systems are commonly needed to concentrate multi-component liquid solutions, suspensions, and emulsions in the food and dairy, pulp and paper, petrochemical, chemical, and pharmaceutical industries. Evaporation systems normally achieve high levels of energy recovery by optimally cascading heat using various multi-effect arrangements [41] as well as heat integration of evaporation/condensation loads with the heating and cooling needs of other processes [42]. Integration of evaporation systems with vapour recompression technologies is a different approach for attaining high levels of energy efficiency, without increasing the number effects. The concept of vapour recompression in evaporation systems is to upgrade low-pressure vapour from an effect's evaporation-side to a higher temperature and pressure for re-injection on the condensation-side of the same or another effect. Mechanical Vapour Recompression (MVR) uses a blower to lift the pressure and temperature of a vapour flow. Thermal Vapour Recompression (TVR) uses a thermo-compressor in conjunction with steam injection for vapour recompression. Of the two techniques, an MVR blower requires higher capital investment, but can greatly reduce the number of effects and lower overall energy use and operational cost [43].

Carrying on from the developments in evaporation system integration for individual unit operations, the contribution in this area [44] introduced a new Total Site Heat Integration (TSHI) method for the design of integrated evaporation systems including vapour recompression that minimises energy use and/or cost objective functions. The design of integrated evaporation systems is a common industrial chemical and process engineering problem. The method defined a new hybrid Total Site Profile (TSP) as a key element of the new design method. This profile forms a composite of nearby streams that may directly integrate with the evaporation system as well as stream segments from processes that require indirect integration via the utility system. The hybrid TSP played an important role in the iterative optimisation of evaporation system design parameters including vapour recompression and evaporation load distribution to optimise objective functions such as total cost, total operating cost, and heat recovery. The new TSHI design method for evaporation systems was demonstrated using an industrial milk processing case study.

4.1.3 Unified Total Site Heat Integration

The following series of work encompassed developed a new Unified Total Site Heat Integration method. These articles comprise the core chapters of a PhD thesis by Mr Amir Tarighaleslami, who recently defended his PhD thesis.

The first of these articles [45] developed a new TSHI targeting methodology that calculated improved TSHI targets for sites that require isothermal (e.g. steam) and non-isothermal (e.g. hot water) utilities. The new method cumulated process level utility targets to form the basis of Total Site utility targets; whereas the conventional method uses Total Site Profiles based excess process heat deficits/surpluses to set Total Site targets. Using an improved targeting algorithm, the new method required a utility to be supplied to and returned from each process at specified temperatures, which is critical when targeting non-isothermal utilities such as hot water. Such a constraint was not inherent in the conventional method. The subtle changes in procedure from the conventional method meant TSHI targets were generally lower but more realistic to achieve. Three industrial case studies representing a wide variety of processing industries were targeted using the conventional and new TSHI methods, from which key learnings were underscored.

A follow-up paper [46] then presented a new Total Site Heat Integration utility temperature selection and optimisation method that optimised both non-isothermal (e.g. hot water) and isothermal (e.g. steam) utilities. Very few existing methods at the time addressed both nonisothermal and isothermal utility selection and optimisation incorporated in a single procedure. The optimisation affected heat recovery, the number of heat exchangers in Total Site Heat Exchanger Network, heat transfer area, exergy destruction, Utility Cost, Annualised Capital Cost, and Total Annualised Cost. Three optimisation parameters, Utility Cost, exergy destruction, and Total Annualised Cost were incorporated into a derivative based optimisation procedure where derivatives may be minimised sequentially and iteratively based on the specified approach. The new optimisation procedure was applied using three different approaches. The merits of the new method were illustrated using the same three case studies as Article 14. Results for the case studies suggested the best derivative optimisation approach is to first optimise Utility Cost in combination with exergy destruction and then to optimise Total Annualised Cost. For this approach, Total Annualised Cost reductions between 0.6 and 4.6 % for different case studies and scenarios were achieved.

The final segment [47] of the series from Mr Tarighaleslami's PhD thesis focused on Utility Exchanger Network Synthesis for Total Site Heat Integration. Although Total Site Heat Integration (TSHI) targeting and optimisation methods have been well developed, few studies had dealt with detailed Utility Exchanger Network design. The Utility Exchanger Network is the

network of heat exchangers that connect a site's centralised utility system to each process while also facilitating inter-process heat recovery. This paper presented a new Utility Exchanger Network design procedure based on the recently developed Unified TSHI targeting method. In the new Utility Exchanger Network design procedure, calculated utility targets from the unified targeting method were achieved after Utility Exchanger Network design and the number of exchangers reduced compared to the design procedure based on the conventional method. are achieved after UEN design based on both design procedures.

4.1.4 Total Site Mass, Heat and Power Integration Using Process Integration and Process Graph

Total Site problems with simultaneous mass, heat, and power integration, i.e. Total Site Mass, Heat and Power Integration (TSMHPI), as shown in [Figure 8,](#page-17-1) has received significantly less attention even though this has been viewed as an area of rich potential for a new generation of mega processing sites.

Figure 8: Total Site Mass, Heat and Power Integration (TSMHPI) problem.

This contribution [48] aimed to develop a novel method to visualise and solve Total Site Mass, Heat and Power Integration problem using a combination of Process Integration and P-graph techniques. The new method incorporated three important process engineering tools: (1) process modelling of mass and energy balance, (2) Pinch Analysis of individual processes and Total Site Heat Integration of clusters of related processes, and (3) the construction of a Total Site superstructure within the P-graph framework to represent the possible mass, heat, and power interconnections between process and utility systems.

4.2 CASE STUDIES

TSHI case studies are divided into three sub-sections covering a total of eight articles. The first section focused on TSHI of milk powder productions that are stand-alone. The second section presents four articles that applied Heat Recovery Loop approach to the site-wide integration of hot water as well as the integration of solar heat. The third and final section presents an article with a biorefinery case study.

4.2.1 Total Site Heat Integration and Optimisation of Milk Powder Production

In the milk powder process, some of the stream data is "soft", meaning that some flow or temperature set points or target values can vary without impacting the process, product quality and safety. Variations to present stream data may be achieved in several ways, such as by applying new control set-points to the existing process. Designers can use this flexibility to their advantage by varying soft data within a defined range to obtain a minimum energy use target. Soft data selection can also significantly impact the development of heat exchanger network structures that are designed to maximise heat recovery.

In the first application [49], TSHI was applied to determine the impact of soft data selection on the Total Site energy targets and the Pinch Temperature of milk powder production. The initial TSHI study highlighted the need to investigate additional process and utility integration opportunities. The study was followed by a detailed analysis and PI integration of the milk evaporation system by the appropriate placement of vapour recompression operations [32]. The opportunity of spray dryer exhaust heat recovery including a detailed and validated model was another important step [34]. After exhausting the energy savings potential within the process system, the follow-up work considered ways to save energy within the utility system through the practical application of condensing economisers and waste heat upgrading and recovery from chillers [50].

The contributions of the integrated process design for the milk evaporation, spray dryer and utility system were then combined to create a new Ultra-Low Energy Milk Powder Production design [51]. It was the capstone of several years progress toward low-energy milk powder production. The basis for the analysis was a state-of-the-art modern milk powder plant that required 5,265 MJ/t_p of fuel and 210.5 kWh/t_p (58.5 MJ_e/t_p) of electricity. The model of the modern milk powder plant was validated against industrial data and changes to process and/or utility systems were targeted and implemented into the model to understand the impacts on thermal and electrical demands and emissions. Results showed that seven significant changes were beneficial: (1) pre-concentration of milk to 30 % using reverse osmosis, (2) a two-stage intermediate concentrate (30 %) homogenisation to enable high solids (60 %) spray drying, (3) an ultra-low energy Mechanical Vapour Recompression evaporator system, (4) spray dryer exhaust heat recovery, (5) condensing economiser for the boiler, (6) upgrade and integration of chiller condenser heat, and (7) recycling of air in the building ventilation system.

These changes were estimated to reduce thermal energy use by 51.5 %, electricity use by 19.0 %, and emissions by 48.6 % compared to a modern milk powder plant. The comparison of energy use by modern (Design 1.0) and ultra-low energy (Design 3.0) are presented in [Figure 9.](#page-19-0)

Figure 9: Sankey diagrams for a modern milk powder plant and an ultra-low energy milk powder plant, comparing energy, water removal, and product flows.

4.2.2 Heat Recovery Loops for Site-wide Dairy Factory Heat Integration

Heat Recovery Loops are often applied to indirectly recover and place heat in processing clusters with processing and Pinch Temperatures below 100 °C [15]. In a Heat Recovery Loop system, an intermediate fluid, usually water, is pumped to plants with excess heat in the desired temperature range to recover heat. The fluid is then piped back to a tank, which acts as thermal storage, before being sent to plants that require heating in the same temperature range. The system is closed and the fluid is continuously circulated depending on the heating and cooling requirements of the various processes. Fluid storage acts as a buffer to mass and enthalpy imbalances between the hot and cold sides of the loop and is ideal for improving HR on large multi-process sites with lots of semi-continuous processes in operation.

The interrelationship between HRL storage temperatures, heat recovery and total HRL exchanger area contain an interesting trade-off [52]. A methodology for designing a HRL based on a ΔT_{min} approach was developed to compare to three programming optimisation approaches where heat exchangers are constrained to have the same Number of Heat Transfer Units (NTU), Log-Mean Temperature Difference (LMTD) or to find the absolute Minimum Total Area (MTA) for a given heat recovery level. The analysis was performed using time-averaged and transient mass flow rate data and temperature data. The actual temperature driving force of the HRL heat exchangers was compared to the apparent driving force as indicated by the Composite Curves. Results for the same heat recovery level showed that the ΔT_{min} approach is effective at minimising total area to within 5 % of the global minimum area approach.

Combining solar heating with Heat Recovery Loops is a cost-effective way to share common storage and piping infrastructure. The conventional HRL design method based on a CTS (constant temperature storage) and a new HRL design method using VTS (variable temperature storage) were applied to demonstrate the potential benefits of inter-plant heat integration and installing solar heating [53]. The dairy case study had available 12 source streams including four spray dryer exhausts and six sink streams. The addition of the dryer exhausts as heat sources was a critical factor in gaining a heat recovery of 10.8 MW for the variable temperature storage design, of which 5.1 MW was contributed from exhaust heat recovery. For the same minimum approach temperature, the variable temperature storage design approach achieved 37 % more heat recovery compared to the constant temperature storage design approach.

Integration of solar thermal energy into low-temperature Pinch processes, like dairy and food and beverage processes, is more economic when combined with a Heat Recovery Loop to form a combined inter-plant heat recovery and renewable energy utility system. The combined system shares common infrastructure such as piping, pumping and storage, and improves solar heat utilisation through direct solar boosting of the HRL intermediate fluid's temperature and enthalpy either through parallel or series integration relative to the other sources and sinks in the HRL system. The three options for integrating solar thermal directly into a Heat Recovery Loop were dynamically modelled using historical plant data from a large multi-plant dairy case study to demonstrate the hot utility savings potential of the solar-HRL system [54]. Case study results showed the best location for integrating solar heating into a Heat Recovery Loop is in series with the heat sources as the hot fluid returns to the storage tank. This configuration maximised the effectiveness of collecting solar heat as a meaningful replacement of non-renewable process heat.

4.2.3 Total Site Utility Systems Design using P-graph

Sustained growth in renewable electricity generation has changed the dynamics of many electricity markets. Large swings between high-peak and low-off-peak electricity prices resulting from the complex interplay between intermittent renewable energy supply, continuously fluctuating electricity demands, and market structure and policy [55]. This contribution [56] aimed to optimise the structural design of industrial central utility systems to take full advantage of intraday electricity spot price fluctuations. Surges in renewable electricity generation uptake have amplified the rises and falls between peak and off-peak electricity prices. Industrial Total Sites and Locally Integrated Energy Sectors can take maximum advantage of periods of both low and high electricity prices through appropriate technology investment.

The historical price in wholesale electricity index for the EU-28 experiences many fluctuations. The median hourly electricity price trend for a daily cycle shows a low trough (4 a.m.) during the night, a small peak in the morning (8 a.m.) followed by a downturn in the afternoon before rising to a high peak in the evening (7 p.m.). The absolute electricity price is heavily influenced by the season as indicated by the individual trends for the different days. Ordering all electricity price provides a sense of the frequency that each price point arises. A three-period approximation of the ordered electricity price profile can be formulated. There is a trade-off between the accuracy of the approximation (i.e. more periods) and the computational burden and is an area that may attract attention in future work.

Using P-graph, a Utility Systems Planner superstructure was developed and extended to apply a multi-period analysis to optimise the selection of the fuels, energy conversion technologies, and the required sizes to install for a representative case study. A key difference between the multiperiod solution and the single-period solution, [Figure 10,](#page-21-0) is an Electric Boiler that operates when the electricity price is low. This resulted in a Total Annual Cost saving of 7.5 %.

Figure 10: Utility systems structural design with key fuel and equipment for minimum Total Annual Cost.

5 MACRO ENERGY PLANNING AND INTEGRATION

5.1 NOVEL AND INNOVATIVE METHODS

The novel and innovative contributions to methodology development in macro-energy systems focus on two areas. The first area is energy planning using Energy Ratios. The second area is targeting localised Waste-to-Energy networks.

5.1.1 Energy Ratio Analysis and Accounting for Renewable and Non-Renewable Electricity Generation

Sustainability metrics and indices are important tools to quantify the environmental, social, and economic impact of industrial processes and human activity [57]. Where economic analyses may be affected and blurred by dynamic market prices, capital cost competition, and government policy, sustainability metrics are established based on fundamental science and engineering principles [58].

The study reviewed and compared five Energy Ratios that may be used in energy planning studies and as sustainability metrics for evaluating common electricity generation methods. The Energy Ratios included Energy Return on Investment (EROI) – standard and external, Energy Payback Time (EPT), Primary Energy Factor (PEF), and Resource Utilisation Factor (RUF). A common energy analysis framework, together with three accounting methods based on energy value, exergy, and primary energy, were described. The concept of the time-value for energy as an analogy to the time-value for money was synthesised into the Energy Ratio calculations.

The analysis framework was implemented in a spreadsheet tool and applied to analyse 45 generation projects. Results for EROI and Energy Payback Time rank nuclear, natural gas CCGT, and geothermal (in Iceland) as the top-performing generation methods with EROI_{ext} values exceeding 30 and Energy Payback Times less than 2.5 months. The second tier of generation performance includes hydro, wind, geothermal (in New Zealand) and coal power stations with EROI_{ext} values of $5 - 30$. Last, solar PV consistently achieves the poorest Energy Ratios with EROI_{ext} values between $0.5 - 7.6$ and significantly longer Energy Payback Times compared to other generation options. Accounting for the time-value of energy has a very significant impact on the calculated Energy Ratios. The energy accounting method has a similarly critical effect. Energy Ratio performance levels for renewable energy generation sources – hydro, wind, geothermal and solar – all rely heavily on the quality of the primary natural resource available. This study concludes that EROIext and Resource Utilisation Factor are the recommended Energy Ratio metrics for inclusion in full sustainability assessment and that it is critically important to account for both energy quality and the time-value of energy.

5.1.2 Networks for Utilising the Organic and Dry Fractions of Municipal Waste: P-graph Approach

Municipal Waste management comprises a number of important activities. The overall management involves a number of steps: collecting the waste from the households or collection points in the neighbourhoods, transportation to transfer stations and/or processing facilities, waste processing – including sorting, separation, treatment, thermal treatment, and anaerobic digestion.

The aim of this work was to apply a new model for preliminary targeting of Waste-to-Energy supply chains. Using the performance targets, the trade-off between the emissions, energy and cost reduction resulting from the potential Waste-to-Energy implementation may be understood, allowing the consideration of lower-scale Waste-to-Energy facilities alongside the large-scale ones. The work built upon the WTE targeting model proposed in Walmsley et al. [59] and extended it by providing a derivation of the underlying targeting model and then applied it to a case study based on a set of price data from official statistical sources and performance specifications derived from the literature. The evaluation scheme investigated the WtE supply chain performance for ranges of area and population sizes and two levels of population density, typical for Europe. The final segment of the study looked to clearly address the challenges posed by the waste logistics and directions for future research. The full journal article that reports this work is currently under review for publication in Frontiers of Chemical Science Engineering.

Figure 11: A visual superstructure of the Waste-to-Energy problem in P-graph Studio

5.2 CASE STUDIES

5.2.1 New Zealand Energy Sector Planning for GHG Emissions Reductions

In a series of three articles, the New Zealand energy sectors of electricity [16], transport [60] and process heat [61] were studied using the lenses of Carbon Emissions Pinch Analysis [10] and Energy Return on Energy Investment analysis [18]. In the first paper [16], Carbon Emissions Pinch Analysis and Energy Return on Energy Investment analysis were combined to investigate the feasibility of New Zealand reaching and maintaining a renewables electricity target above 90 % through to 2050, while also increasing electricity generation at an annual rate of 1.5 % and allowing for a 50 % switch to plug-in electric vehicle transportation for personal use vehicles. Under this scenario, New Zealand's electricity demand was anticipated to reach a maximum of between 70 and 75 TWh by 2050. Future electricity generation planning solutions were based on a simple optimisation method. For different carbon emissions cap, the electricity generation mix that gave the lowest total energy investment was determined.

If New Zealand forced to achieve the 1990 carbon emissions level of $3,730$ kt CO₂-e in 2050, electricity growth will need to come from wind (18 TWh) and geothermal (13 TWh), and hydro (5.6 TWh). This combination of sources minimised the energy investment required from the economy. Renewable resources were needed to produce close to 95 % of electricity generation. The analysis demonstrated that New Zealand is in a very good position to sustainably meet the future electricity needs while maintaining very low carbon emissions levels and economically desirable Energy Return on Energy Investment levels.

In the second paper of this line of work [60], the Carbon Emissions Pinch Analysis method for energy planning was modified for improved application to transport energy sectors. The modified method was applied to investigate the feasibility of New Zealand reaching a 1990 emission level for transport by 2050. The transportation sector has been traditionally a difficult area to transition to high levels of renewable energy because of the strong dependency on fossil fuels.

Using the Carbon Emissions Pinch Analysis composite curve method, the freight and passenger transport demand in New Zealand for the year 2012 were developed. Results showed passenger transport contributes 12% of the useful transport output but is responsible for 71% of transport emissions. The total freight transport demand and emissions for NZ in 2012 were 95.9 Mt-km and 5.0 Mt CO₂-e respectively (Transport Emission Factor: TEF = 0.052 Mt CO₂-e/Mt-km). The total passenger transport demand and emissions for NZ were 13.1 Gt-km and 12.4 Mt $CO₂$ -e respectively (TEF = 0.944 Mt CO₂-e/Mt-km). In both cases the amount powered by renewable fuels was negligible.

Factors vary depending on the freight or passenger load factor, engine technology and tare weight differences rather than fuel differences. Marine transport is clearly very efficient at transporting both freight and people with marine vessels having the lowest emission factors in both demand classes. Freight rail is equally a low emissions transport method and road freight methods are the highest. It is important to note that although road freight methods have the highest emissions factors, they have additional cost benefits of being flexible giving point-to-point delivery with minimal handling stages.

With passenger transport, Light Personal Vehicles – LPV stands out as generating 65% of passenger transport emissions while delivering only 28% of the useful transport output. High Factors for rail and bus are principally caused by low participation rates as a result of high LPV use, and as a result, the useful transport output from these classes is relatively small. Air transport, including domestic and international travel, contributes 27% of passenger transport emissions and provides 25% of the useful transport output.

For New Zealand, identified steps for low carbon emissions from transport were: (1) the electrification of all rail, (2) the widespread adoption of energy efficient vehicle technologies, (3) the partial electrification of light passenger vehicles through plug-in hybrid and electric vehicle technologies, and (4), the introduction of liquid fuels from biomass as an alternative to liquid fuels from petroleum.

In the final segment of the series, options for reducing industrial process heat GHG emissions in New Zealand were investigated in this paper using the Carbon Emissions Pinch Analysis and Energy Return on Energy Invested analysis methods. Renewable sources like geothermal, biomass, biogas from animal waste and heat pumps from renewable electricity were spatially plotted on a map of New Zealand to understand the locations of energy resources and demands. Results indicated that some regions of New Zealand were well placed to make significant reductions to process heat GHG emissions through shifting from fossil fuel heating to renewable heating without a large increase in energy investment. Reducing GHG emissions below 1990 levels could be achieved by using wood waste and biomass in place of coal (33.3 PJ) and biogas from animal waste in place of natural gas (12.1 PJ) where high-temperature heating is required ($>90^\circ$ C), and renewable electricity driven heat pumps for low temperature heating ($\leq 90^\circ$ C) in dairy and meat processing industries (7.0 PJ). The expected increase in required energy investment was 20 %.

5.2.2 Energy Return on Energy and Carbon Investment of Wind Energy Farms: A Case Study of New Zealand

Consistently high average wind speeds are critical to making wind an economically viable generation option. New Zealand has access to excellent wind resources. For example, the Cook Strait and Manawatu gorge, in the south of the North Island, channels strong winds creating prime locations for electricity generation. Most New Zealand wind energy farms operate at capacity factors greater than 30 %, with some individual turbines achieving over 50 %. For comparison, Denmark experiences slightly lower capacity factors of $25 - 30\%$ [62]. The average capacity factor for wind energy farms in Europe is 21 %, with the highest being 57.9 % [63].

Economic analysis of wind energy potential in New Zealand is favourable for many sites. The Long Run Marginal Cost of wind and geothermal is between 80 and 100 NZD and are the two lowest cost options for new electricity generation [64]. New Zealand has an open market with no direct subsidies or incentives for renewable generation other than the Emissions Trading Scheme, which requires electricity companies to purchase carbon credits equal to the quantum that is emitted, and market forces. A Government ministry commissioned study projects up to 6,600 MW of wind energy may be available across the nation [65] but not all of this potential will be economic.

The work in on wind energy in New Zealand [66] analysed the Energy Return on Investment and Energy Return on Carbon Emissions of current wind energy farms in New Zealand. The weighted average EROI for a New Zealand wind energy farm over a 20 y lifespan was 34.3, with the highest achieving 57.7, while the lowest was 6.5. These values were higher than wind energy farms in Europe and America, which average about 20, and higher than many other electricity generation methods reported in the literature with hydropower being the main exception. The above-average capacity factor of New Zealand wind energy farms is the primary reason for the higher Energy Return on Investment values. The average Energy Return on Carbon Emissions value for New Zealand's existing wind energy farms is $477 \text{ GJ/t } CO_2$ -e, which is 56 times the value of a combined cycle natural gas power station. The substantial range of Energy Return on Investment values was chiefly driven by two factors: (1) wind speed profile for a given site and (2) the blade diameter of the turbine, where greater values are better. The main drawback of wind energy remains its variability causing reliability issues and needing hydropower as a renewable buffer to maintain low emissions.

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