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Data Extraction for Heat Integration and Total Site Analysis: A Review

Petar Sabev Varbanov[a,*], Jun Yow Yong[b], Jiří Jaromír Klemeš[a], Hon Huin Chin[a]

[a]Sustainable Process Integration Laboratory – SPIL, NETME Centre, Faculty of Mechanical Engineering, Brno University of Technology - VUT Brno, Technická 2896/2, 616 69 Brno, Czech Republic
[b]Faculty of Information Technology, University of Pannonia, Egyetem u. 10, Veszprém, Hungary
varbanov@fme.vutbr.cz

This work discusses a crucial activity for Heat Integration (HI): Data Extraction (DE). Overall, data acquisition is a complex process involving many stages and stakeholders. The paper analyses the treatment of DE in the published literature. The analysis established that many publications just present the results from already performed DE and others limit the provided reasoning only to a few key issues. Further, the importance of the preservation of data integrity and semantics is highlighted. This can be done by documenting the reasoning and the choices made during DE, as well as distributing the DE reasoning between the general discussion and stream-specific information placement into the Process Streams Table for HI, preserving the context. The approach is illustrated on a published example.

1. Introduction

HI is the foundational Process Integration (PI) part, for which DE has a crucial significance (Klemeš et al., 2018). The adequacy and quality of the proposed solutions depend on selecting the right data set, which captures all relevant heating and cooling demands of the considered process. If some of them are missed, the engineers would be solving a wrong HI problem (Rossiter, 2010). On the other hand, certain streams on a site should not be extracted for integration for safety reasons – for instance, parts with high explosion risk (Chew et al., 2013). Another essential aspect of DE is the complex nature of the activities and the data flow (Matsuda et al., 2009). The activity involves several different stakeholder types, exchanging data. Advanced software can be used to preserve the data continuity – as can be seen from a case study on a crude oil refinery (Cui and Sun, 2017). However, a significant role in the data sets is played by semantics. All stakeholders have to reach a common understanding on the reasons for streams selection. Without that, mutual control and feedback are impossible, which reduces the level of confidence in the data quality. This brings the need to establish a common format and rules for composing datasets for HI. This format has to contain, in addition to the data, a set of descriptors of the reasoning for selecting and excluding the streams and their parameters.
The current contribution reviews the HI and DE developments in the literature and some research and demonstration projects. It formulates a set of data requirements for DE systematically, enabling the development of an appropriate data format. The discussion is illustrated with a published case study (Varbanov et al., 2006).

2. Review of Data Extraction treatment in the literature

Several key books have treated DE. The “User Guide” by Linnhoff et al. (1994) has been the cornerstone of teaching HI, providing complete HI instruction with conceptual discussions, Batch HI, Distillation Column Profiles, low-temperature processes, water/wastewater minimisation, Total Site, emissions targeting. It discusses the DE principles, emphasising the importance of solving the right problem. The discussion starts with data accuracy, advising to strive for more accurate data only in the vicinity of the Pinch. It is explained how to choose the Heat Integration Process Streams, including a selection of genuine heating and cooling requirements, “soft temperatures”, and avoidance of non-isothermal mixing.

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The Handbook of Process Integration (Klemeš, 2013) treats DE in Chapter 4. It focuses on explaining the DE rules applied in practice and the reasons for instituting them, elaborating on the stream mixing, practical constraints and soft data. Chapter 36 of the PI Handbook (Klemeš, 2013) presents a focused discussion and a systematic consideration of the DE rules and their implications. DE is considered within the context of the overall workflow for performing a study for increasing the heat recovery of an industrial process. The core rules have been thoroughly examined and explained. These include when to extract heating/cooling requirements, data precision, heat capacity variation handling, temperature and load selections, cost data. These traditional considerations have been supplemented by a short analysis of DE for the integration of renewable energy sources, resulting from their intermittency.

Savulescu and Alva-Argaez (2008) investigated the additional opportunities for heat recovery improvement in Kraft paper mills, that arise by including Direct Heat Transfer (DHT) in the analysis. The discussion starts with the classification and description of the DHT types in the process. It further analyses the process operations involving DHT – such as pulp dilution, questioning the need and extent of the heat transfer. The authors provide further analysis of the DE options, assuming a retrofit situation, aiming to minimise the DHT operations and eliminate Cross-Pinch heat transfer caused by the mixing.

Al-Riyami et al. (2001) have considered a real refinery case study, focusing on the HI of a Fluid Catalytic Cracking plant. They used a process simulator for establishing the flowsheet, mass and energy balances. The paper provides a summary of the incurred DE issues, pointing out certain parts of the process excluded from the selection. However, as the focus of the article is the illustration of the Heat Exchanger Network (HEN) retrofit procedure, achieving 27 % utility cost savings at 1.5 y payback time, no further details on the DE are provided.

A case study on the HI of a process for bio-ethanol production (Kravanja et al., 2013) provides a brief representation of DE reasoning, typical for published heat recovery studies. It lists the extracted process streams with their temperatures and loads, and a summary of which heating or cooling demands have been included in the data set and which have been left out. The reasons for those choices are not discussed.

An evaluation of the HI opportunities for a palm oil processing plant (Lidu et al., 2016) starts with establishing the flowsheet and providing a description of the process and the main parameters in terms of temperatures and flowrates. The DE is then presented by listing the extracted process streams, briefly explaining the choice of temperature for one of the streams and documenting the exclusion of two other streams from the selection.

A Grid Diagram variation focusing on path tracing for HEN retrofit has been presented in (Nemet et al., 2015). The paper examines a HEN retrofit study, starting from the process identification, proceeding to balancing, DE and Data Reconciliation (DR), retrofit targeting, analysis of the current HEN for retrofit options, and recommending retrofit actions for improved heat recovery using the newly developed Retrofit Tracing Grid Diagram. The DE section of the article summarises the DE rules as applied to the particular case study.

A biomass gasification case study is presented in (Pavlas et al., 2010). The process also has an integrated scrubber for the synthesis gas cleaning. The study evaluated the HI options, also considering a heat pump. The evaluation found an opportunity for economically justified electricity generation. Within the case study, the DE is represented only by the identified HI Process Streams. Pouransari et al. (2014) provide a discussion on how to perform DE for HI at various levels – from a single process up to the site level. They consider top-down and bottom-up options. While the considered options are valid and important, no clear interface between the process energy demands can be identified, which would allow performing a practical HI analysis.

The importance of safety considerations in DE is discussed in (Varbanov et al., 2016). Since HI increases the complexity of the process – in terms of management and control, certain process parts should be left out of the integration, allowing isolation and efficient management of the related process risks. Wan Alwi et al. (2014) have also added into the HI studies consideration of heat losses and heat gains that take place due to differences of the stream temperatures and the ambient temperature. They reason that the data to be extracted should also include the ambient conditions and heat transfer coefficients of the pipe and equipment casings.

Data integrity can be preserved within a single software suite. This can be seen on the example of the case study on a crude oil refinery (Cui and Sun, 2017), where the initial flowsheets have been balanced and simulated in Aspen Plus (2019), then the DE has been performed using Aspen Energy Analyzer (2019). While such an automated DE may capture most of the relevant process streams, it would still be missing the careful consideration by engineers and the relevant reasoning that should be kept together with the complete documentation in a PI project.

3. Data Extraction – analysis and suggested improvement

A couple of patterns emerge from the review in the previous section. Rules and guidelines for DE have been well formulated for HI studies in the “User Guide” (Linnhoff et al., 1994) and the PI Handbook (Klemeš, 2013). They have become a mandatory part of authoritative PI books – including the book on the PI approach to

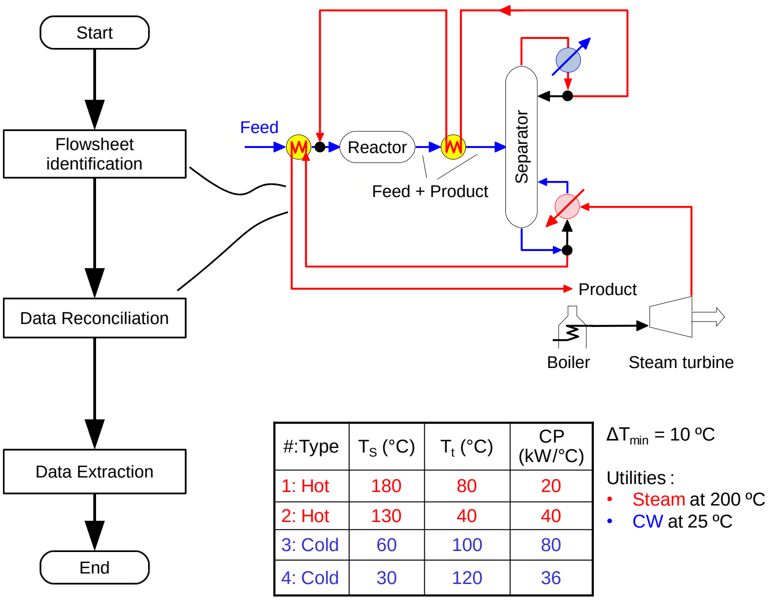
Chemical Process Design (Smith, 2016) and the recent PI-focused textbook discussing energy and water integration, and power planning (Klemeš et al., 2018). There have been other follow-up developments to the “User Guide” (Linnhoff et al., 1994). These include a systematic procedure for embedding DE into HI workflows (Klemeš and Varbanov, 2010) and an extension to handle cases of DHT (Savulescu and Alva-Argaez, 2008). Some works have presented DE to a varying degree in their HI case studies. In some, only the results of the DE are presented in the typical tabular form, as in (Pavlas et al., 2010). Other provide DE reasoning limited to specific issues excluding process streams from selection (Al-Riyami et al., 2001) or provide more complete reasoning in the case analysis description (Kravanja et al., 2013).
The discussed sources do provide useful information and examples. However, for industrial-scale case studies, the data acquisition process should be considered systematically – preserving the continuity and the semantics of the performed evaluation. Such a consideration was not found in those works and the literature, associated with the term “Data Extraction”. This section fills in the gap by proposing one way of preserving the continuity and the integrity of the extracted data, together with its associated semantics and related reasoning.

3.1 Site- and process-level procedures

The data acquisition for a HI evaluation most often starts at the site level and follows the steps:

1) Site Description
2) Identification of potential interfaces
3) Scoping site processes
4) Data acquisition for each selected process

The first step involves obtaining a description of the site, including an overall diagram of process connections and the utility system, main parameters – as processing capacities, process energy demand, primary energy demand, heat and power generation and waste energy flows. The potential interactions of the site with the surrounding regional and municipal entities can be evaluated for increasing the efficiency of the energy resource utilisation via any waste heat reuse. A typical scheme of this type is the potential to supply district heating to nearby residential demands using industrial waste heat. The further step is to perform process scoping, determining which site processes to include for further considerations. This selection can be made based on site steam system evaluation for potential cost savings – as done in Top-Level Analysis (Varbanov et al., 2004) or safety considerations (Varbanov et al., 2016). The last stage is performed for each of the selected processes. It identifies the process flowsheets, then the stream properties, and the data are processed with DR to ensure consistency, followed by the DE, proceeding in two parts. First, the current (existing) duties of the heat exchangers, heaters and coolers are identified. This provides a baseline for the follow-up heat recovery evaluation. The second part of this procedure is the Process Streams selection for HI.



#:Type	T_S (°C)	T_t (°C)	CP (kW/°C)
1: Hot	180	80	20
2: Hot	130	40	40
3: Cold	60	100	80
4: Cold	30	120	36

Figure 1. Data acquisition for a process

In acquiring the data for each process, it is vital to ensure several properties of the treated data set: continuity, clear links between objects that are linked in the real process, data consistency and adequacy for calculation and decision-making, conformance to the interfaces of the applied methods. The data acquisition workflow at the process level is shown in Figure 1. The first step is to establish the process flowsheet – the set of process operations involved, their connections and the streams implementing the connections. This should also be accompanied by the appropriate mass and energy flow measurements and approximate balancing. The next step is the DR. This activity ensures consistency of the measured data (Veverka and Madron, 1997). It uses the measured data for flowrates, temperatures, pressures, together with the appropriate process constraints, to reconcile the data set, ensure its consistency and fidelity. The next step is the DE for HI that uses the Reconciled Data Set.

Considering Figure 1, it can be noticed that the workflow refers to several data sets: (a) the flowsheet showing the operating units, flowsheet streams and their properties; (b) the Reconciled Data Set; and (c) the HI problem data set. The data continuity and consistency have to be kept among these data sets. Using appropriate software tools – e.g. Aspen Energy Analyzer (2019) these properties are ensured.

However, there is one more property, that is important to preserve across all data sets in the workflow. This is the continuity of the data semantics, which includes the chain of reasoning applied to obtain each following data set from the previous. While DR is automated to a large degree, applying an agreed and unified mathematical model, the DE stage is subject to engineering judgement. The chain of reasoning should be recorded, linking the Reconciled Data Set and the data set for the HI Process Streams. An example of more subtle reasoning, which requires judgement, is the case of the high-temperature waste heat, usually available from hydrogen production units in petroleum refineries. Some engineers may suggest using this waste heat, as it is also available in substantial amounts. However, refinery site engineers are reluctant to consider such an option, due to the high risk of explosion, which leaves this type of waste heat out of the process/stream selection for HI.

One way to allow for such continuity and integrity is to provide the appropriate reasoning for the selection of the Process Streams in two places:

(a) The general discussion should be placed in the main text of the document – report or article. This should also include a table of streams excluded from the HI, with explanatory notes.

(b) The stream-specific information should be provided in the Process Streams Table (Table 1).

This arrangement provides a right balance and a hierarchy for recording the course of the DE and allows to easily trace any decisions made, and to efficiently make changes to those choices during project iterations. In Table 1, the unit for temperature is K because the illustrative example uses this. Using °C is usually preferred.

Table 1. Template for an enhanced Data Extraction format

#	Name	Flowsheet IDs and links	T_S (K)	T_T (K)	ΔH (kW)	CP (kW/K)
Number	An informative process stream name for the HI context	An identifier of a flowsheet stream or identifiers of a linked group of streams	Supply Tempe-rature Value	Target Tempe-rature Value	Enthalpy Change (flow) Value	Heat-Capacity Flowrate Value
	Description of the selected context and reasoning					

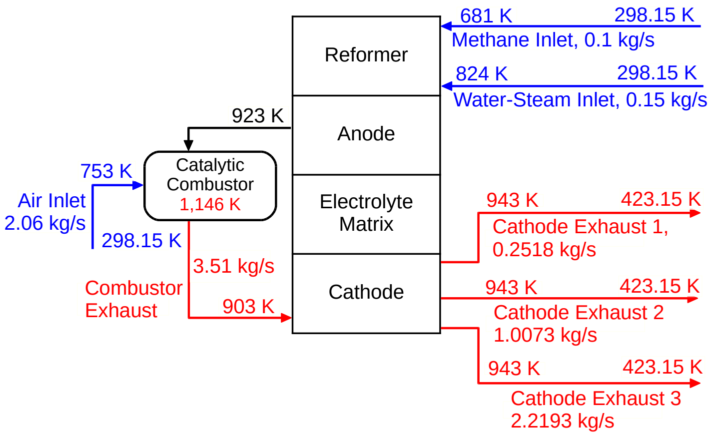


Figure 2. MCFC Flowsheet, adapted from (Varbanov et al., 2006)

3.2 Illustrative example

To show a potential implementation of the proposed integrity preservation approach, the example from the Fuel Cell HI, discussed in (Varbanov et al., 2006), is used. That study considered a Molten Carbonate Fuel Cell (MCFC) and studied the opportunities for maximising the utilisation degree of the spent fuel. It combines the MCFC with a HEN for recovering the maximum amount of heat and generating steam, which is then passed to a steam turbine, generating additional power. This allows increasing the power generation efficiency from that of the MCFC (46.38 %) up to the Fuel Cell Combined Cycle – to nearly 70 % (between 60.23 % and 69.38 %). The HI study starts with the DE from the MCFC flowsheet (Figure 2), assuming that the data are reconciled.
The DE reasoning starts with an overview of the flowsheet streams and reasoning for selecting each of them for HI or not. The anode exhaust, with temperature 923 K, is sent to the catalytic combustor, to complete the combustion of the excess fuel. It does not undergo heat exchange, so it is left out of the selection. The rest of the streams have been found to need heat exchange and have been selected for HI (Table 2). The flowsheet identifier (column "Flowsheet ID") and the reasoning for the stream inclusion and parameter selection are added to the traditional HI table format.

Table 2. HI Process Streams selected and the reasoning for the case study

#	Name	Flowsheet ID	T_S (K)	T_T (K)	ΔH (kW)	CP (kW/K)
1	C1	Methane Inlet	298.15	681	109.5	0.2858
The methane gas/natural gas is fed to a reformer to undergo indirect reforming. It is taken from the ambient temperature of 298.15 K. It needs to be preheated to 681 K before it is injected to react with the steam feed.						
2	C2	Water-Steam Inlet	298.15	824	282.7	0.5374
The water from the supply system enters the fuel cell reformer as steam and reacts with methane to undergo a steam reforming reaction. It is supplied at ambient temperature (298.15 K) and preheated to 824 K.						
3	C3	Air Inlet	298.15	753	976.7	2.1465
The exhaust from the anode (mainly CO, CO_2 and H_2O) is burned with the presence of air in the catalytic combustor. The air is heated from the ambient temperature (298.15 K) to 753 K before entering the combustor.						
4	H1	Combustor Exhaust	1,146	903	-1,279.1	5.2638
The combustor exhaust (mainly N_2, CO_2, unreacted CO and O_2) has to be cooled before it is introduced into the cathode. At high temperature, evaporation of electrolyte and corrosion of material are more likely to occur. In this case, it is required to be cooled from 1146 K to 903 K.						
5	H2	Cathode Exhaust 1	943	423.15	-130.9	0.2518
The cathode exhaust consists mainly of N_2, CO_2 and O_2, with traces of SO_2. It is vented to the ambient through a stack. It should be cooled from 943 K to 423.15 K. In the particular device design, it is split into three branches. This is the first branch						
6	H3	Cathode Exhaust 2	943	423.15	-523.6	1.0073
This is the second branch of the cathode exhaust						
7	H4	Cathode Exhaust 3	943	423.15	-1,153.7	2.2193
This is the second branch of the cathode exhaust						
Convention: The heating demands are assigned positive values for ΔH, and the cooling demands are negative.						

4. Conclusions

The current paper has analysed the DE procedure and practices in the published literature. It has been established that, despite the availability of numerous studies, applying HI at the process and site level, there has been little or no discussion on the preservation of the integrity and traceability of data and reasoning. As a result, most of the available HI examples either omit the DE reasoning or provide only highlights.
The information integrity and traceability are essential for industrial-scale projects, as they usually involve a large number of stakeholders from at least two categories – an industrial operator (client) and a consultant. The stakeholders work in a distributed way and play different but linked parts. Integrity preservation is important, to ensure that all parties reach a common understanding. The proposed data set format change illustrates one possible way of ensuring data integrity and traceability for selecting the HI Process Streams in DE.
Based on this understanding, future work in this field should focus on the analysis of the HI workflows and resource efficiency optimisation, to develop a better understanding of the needs for information integrity at all stages. This follows from the iterative nature of industrial projects, where the results at one iteration often reveal the need to alter certain assumptions or measurement values or run re-calculation or re-optimisation loops.

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