Systems & Control Transactions

Original Research Article
Peer Reviewed Conference Proceeding
ESCAPE 36 - European Symposium on Computer Aided Process Engineering
Sheffield, UK. 21-24 June 2026

Work and Heat Exchanger Networks as a General Energy-Integration Strategy for Chemical Processes

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ABSTRACT

The integrated recovery of heat and mechanical work has gained increasing importance in process integration due to the strong thermodynamic coupling between temperature and pressure changes in many industrial systems. This work presents a rigorous framework for the simultaneous synthesis of Work and Heat Exchanger Networks (WHEN), in which heating, cooling, compression, expansion, throttling, and pumping are optimized in a coordinated manner. The problem is formulated using Generalized Disjunctive Programming (GDP), allowing the explicit representation of alternative thermodynamic paths, phase-dependent behavior, and logical equipment choices. Process streams are defined by supply and target states, while only bounds are imposed on intermediate pressures, temperatures, and flow rates. Streams may change classification between hot and cold multiple times and may undergo several phase transitions.Rigorous thermodynamic correlations obtained from Aspen HYSYS are embedded in the optimization model, enabling a physically consistent treatment of condensation, vaporization, and isenthalpic valve expansion without restrictive assumptions. The heat exchanger network is represented implicitly through the Pinch Location Method, avoiding the combinatorial complexity of explicit exchanger matching while accommodating multiple utilities and unclassified streams.The approach is demonstrated through a self-refrigerated alkylation process case study. The optimal solution reveals a non-intuitive thermodynamic path involving alternating vapor and liquid compression stages and multiple phase changes, which enhances internal heat recovery. Compared to a conventional design strategy, the proposed framework reduces total annual energy integration costs by 12.5%. The resulting nonconvex MINLP is solved to global optimality within seconds, demonstrating both robustness and computational tractability.

Keywords: Work exchanger networks, Heat exchanger networks, WHEN, Energy efficiency, Process Integration

INTRODUCTION

In recent years, the integrated treatment of heat and work recovery has emerged as a key topic in process integration, motivated by the need to further reduce energy consumption and carbon emissions beyond what can be achieved through conventional heat integration alone. While classical Heat Exchanger Network (HEN) synthesis focuses on the recovery of thermal energy and Work Exchange Network (WEN) synthesis addresses the reuse of mechanical energy, many industrial processes exhibit strong thermodynamic coupling between heat and work. This coupling has led to the development of Work and Heat Exchanger Networks (WHEN), in which heat and shaft work are considered in a coordinated and sequential manner rather than as independent subsystems [1].

The relevance of WHEN becomes particularly evident in processes involving significant pressure changes, such as gas processing, refrigeration and liquefaction systems, air separation units, and high-pressure chemical reactors. In these systems, compression and expansion steps not only consume or produce mechanical work but also generate substantial temperature changes. As a result, decisions related to pressure manipulation directly affect the thermal structure of the process and, consequently, the opportunities for heat recovery.

According to Haoshui et al. [1] The systematic integration of power and heat has evolved significantly over several decades, moving from basic component design to complex network synthesis. In 1983, the principles of Pinch Analysis were expanded through the "appropriate placement" concept, allowing for the strategic integration of heat engines and heat pumps [2]. This conceptual framework was further formalized in 1987 through the development of a superstructure-based optimization model for the integration of these thermal machines [3].

The specific concept of Work Exchanger Networks (WENs) was formally proposed in 1996 [4], marking a shift toward treating work as a primary utility. In 2007, the ExPAnD procedure advanced the field by combining heuristics, pinch, and exergy analyses for subambient design [5]. By 2014, the field matured into the simultaneous design of Work and Heat Exchanger Networks (WHENs) through superstructure-based MINLP optimization [6].

Recent advancements have focused on refining these synthesis methods to handle increasing complexity. In 2015, new insights regarding the appropriate placement of compressors and expanders led to the development of manual design procedures [7–10]. This was followed by the introduction of an extensive superstructure for WHENs. Perhaps the most comprehensive superstructure is attributed to Nair et al. [11]. In their model, streams are not pre-classified as hot or cold, or as high-pressure or low-pressure. Instead, the model determines their behavior, which may even change across the various stages a stream can undergo between its supply and target conditions. Furthermore, unlike previous models, it accounts for liquid-vapor phase changes. However, it only considers the use of turbines, compressors, and valves, omitting pumps to increase liquid pressure (for instance, in systems that favor condensation prior to pressure elevation to avoid the use of costly compressors).

WHEN FRAMEWORK

The WHEN problem we are dealing with can be stated as follows:

Given a set of process streams with specified supply and target states (pressure, temperature, and phase), the objective is to determine the optimal thermodynamic path for each stream—incorporating heating, cooling, compression, and expansion stages—to synthesize a network of pressure-change equipment, heat transfer units, mixers, and splitters. This configuration is optimized based on a relevant performance metric, such as minimum energy cost, minimum total annualized cost, or minimum total exergy consumption.

Several relevant features address and overcome common limitations in existing models:

- Variable Bounds: The values for state variables (P, T) or flow rates do not need to be fixed beforehand; only the lower and upper bounds for these parameters are required.
- Stream Classification: Whenever possible, streams are pre-classified as hot (requiring cooling) or cold (requiring heating) to improve the numerical performance of the model. If the behavior is unknown a priori, streams can be defined as "unclassified, " allowing the optimization to determine their role.
- Variable Thermodynamic Paths: Streams undergoing both temperature and pressure changes may follow complex routes involving compressions, expansions, heating, or cooling. Consequently, their behavior may switch between "hot" and "cold" multiple times along the path. Therefore, these streams are generally treated as "unclassified."
- Phase-Independent Pressure Changes: Pressure changes are not restricted to gaseous streams (a common simplification in many models); the model includes also liquid compression and expansion through valves, which may result in liquid-vapor mixtures.
- Rigorous Thermodynamic Correlations: The thermodynamic behavior of each stream between its supply and target states is rigorously correlated using Aspen HYSYS. Integrating these correlations into the optimization model provides a realistic, physically consistent description of process behavior, which is particularly important for streams undergoing condensation, vaporization, or significant density variations.
- Isenthalpic Valve Expansion: Expansion through valves is assumed to be isenthalpic. By utilizing rigorous correlations, it is unnecessary to assume constant Joule-Thomson coefficients or to restrict valve expansion to temperatures below the inversion point. Besides, expansions that end in a multiple phase state can be also incorporated (i.e. typical in refrigeration cycles)
- Multiple Utilities: The model allows for the simultaneous use of multiple hot and cold utilities.
- Multistage Compression: If multistage compression is required, it emerges naturally as a result of the optimization process.

Superstructure and model formulation

The overall WHEN model is formulated using Generalized Disjunctive Programming (GDP), which provides a rigorous mathematical structure to represent logical conditions, operational modes, and phase-dependent behavior.

Process streams are allowed to undergo

compression, expansion, throttling, or pumping across multiple pressure-change stages, potentially accompanied by condensation and/or evaporation. Indeed, a single stream may experience several phase changes as it evolves from its initial to final conditions. This behavior is represented through a stage wise model of pressure-change units, schematically shown in Figure 1. Each stage may include compressors, turbines, pumps, and valves. Compressors and turbines operate with vapor-phase streams, while pumps are restricted to liquid-phase segments. Valves may handle vapor or liquid feeds; in the latter case, partial or total condensation may occur due to isenthalpic expansion. A bypass option represents cases in which a stage does not require pressure modification. The outlet of each pressure-change stage is subsequently sent to the Heat Exchanger Network for potential heat recovery or rejection, as indicated in Figure 1

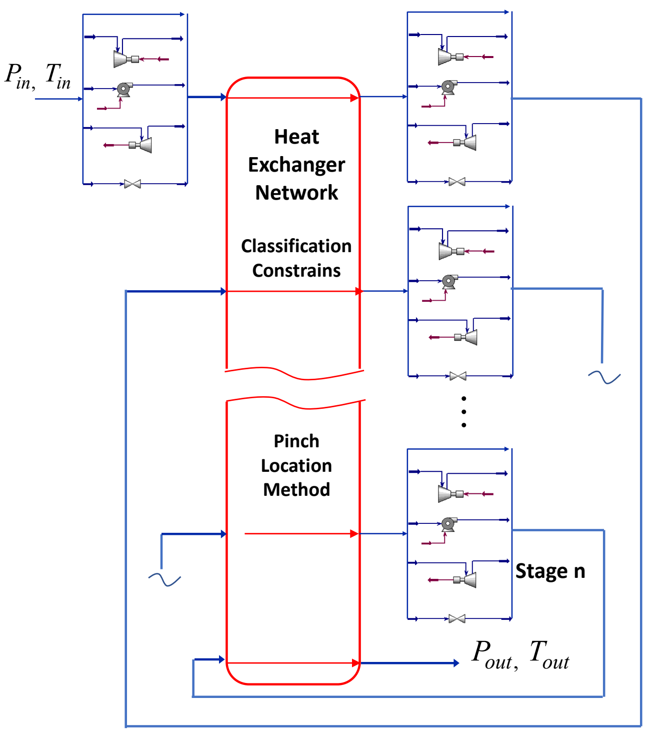

Figure 1. WHEN Superstructure involving streams with change in temperature and presure.

Each stage of a process stream is described as a five-term disjunction, in which each term includes a rigorous model for each one of the possible equipment involved: compression, assumed isentropic with fixed efficiency; expansion in a turbine, also isentropic with fixed efficiency; throttling through a valve assumed isenthalpic; liquid pumping assuming constant liquid density calculated at the inlet conditions; or bypass that simple equals inlet to outlet state variables.

The heat exchanger network itself is not modeled explicitly as a set of predefined exchanger matches, as this would lead to an intractable number of discrete combinations, especially when stream classification and phase behavior are uncertain. Instead, the network is represented implicitly through the Pinch Location [12, 13] Method, which efficiently handles variable heat loads, flexible temperatures, unclassified streams, and multiple hot and cold utilities without enumerating individual exchangers.

Case Study

To illustrate the model, a case study was conducted using data extracted from the process flowsheet presented by Luyben [14] for the self-refrigerated alkylation of C4 olefins with isobutane to produce high-octane C8 components.

In this process, the alkylation reactions occur in a series of stages, which are typically simulated using boiling continuous stirred-tank reactors (CSTRs) such that the reaction product is in the vapor phase. The pressure of this stream must be increased, in this case from approximately 300 kPa to 1480 kPa, for introduction into the separation system. Given that the energy required to compress vapor is significantly higher than that required for liquid compression, and that compressors are among the most expensive equipment in the chemical industry, standard practice involves either condensing the vapor and pumping the resulting liquid or—if the condensation temperature is too low—utilizing a compressor until the condensation temperature is high enough to allow for condensation and subsequent liquid pumping. The original flowsheet uses this second approach.

While this strategy is conceptually sound, it does not account for the potential benefits of integration with the remainder of the process.

Table 1 presents the data for process streams with temperature changes only. Table 2 shows the available utilities while Table 3 details the streams involving simultaneous pressure and temperature changes.

Costs for compressors, turbines, pumps, and other equipment in the optimization model are correlated using the procedure by Turton et al. [15]. Efficiencies for compressors, turbines, and pumps are set at 75%, consistent with the Aspen.Hysys default values.

Table 1. Data for streams without pressure change.

Name	Tin (°C)	Tout (°C)	FCp (kW/°C)
H1	47.01	45.77	130.887
H2	83.26	47.22	7.342
H3	74.19	47.63	245.313
H4	47.22	37.22	63.25
C1	80.69	83.26	75.714
C2	62.56	82.26	367.980
C3	21.00	36.67	28.469

Table 2. Data for available utilities.

Name	Tin(°C)	Tout (°C)	Cost (k$/kW·y)
LP-Steam	120	119	666.4
Water	20	30	20.0
Refrig.	1	5	100
Electricity			1500
Minimum Approach Temperature (ΔT_{min}) = 10 ºC			

Table 3. Data for streams involving simultaneous pressure and temperature changes.

Stream name	St1
Supply Temperature (ºC)	20
Target Temperature (ºC)	75
Intermediate WEN Stages temperature bounds (ºC)	15 – 100
Supply Pressure (kPa)	299.2
Target Pressure (kPa)	1480
Intermediate WEN Stages Pressure bounds (kPa)	250-1500
Supply Phase	Vapor
Target Phase	Liquid
Mean molar liquid density (kmol/m^3)	9.871
Number of WEN Stages	3
Flow (kmol/h)	225.9
Composition (molar fractions)	
Propane	0.1230
i-Butane	0.8415
n-Butane	0.0351
2, 2, 4-Mpentane	0.0004

The optimal solution includes the selection of hot and cold utilities, energy costs (thermal and electrical), and the annualized costs of pressure-change equipment (pumps, turbines, compressors, and drivers); however, it excludes the heat exchanger network (HEN) investment. Once all stream temperatures and flows are determined, designing a HEN that meets all requirements is relatively straightforward.

A simplified flowsheet identifying the process streams involved in the heat and work exchange network is shown in Figure 2.

The optimal solution includes the selection of hot and cold utilities, energy costs (thermal and electrical), and the annualized costs of pressure-change equipment (pumps, turbines, compressors, and drivers); however, it excludes the heat exchanger network (HEN) investment. Once all stream temperatures and flows are determined, designing a HEN that meets all requirements is relatively straightforward. Figure 3 presents the optimal configuration, including the pressure-change equipment for the relevant streams.

The optimal solution shows counterintuitive behavior. Initially, the vapor stream is compressed to the minimum pressure required for condensation with available cold utilities (~309 kPa at approximately 15 ºC). Compression then continues using a liquid-phase pump. However, instead of reaching the final target pressure, the stream is only pumped to ~937 kPa, where it is evaporated and superheated by process streams. A second compressor then raises the pressure to the final specification. This final compression also increases the temperature to approximately 15 ºC above the target temperature.

The second condensation together with the final superheating are used by the system to increase the degree of heat integration, reducing both hot and cold utilities.

The total energy integration cost using the strategy described above is 4, 395 k$/y. In contrast, following the strategy presented by Luyben [15] results in a cost of 4, 945 k$/y, which is 12.5% higher. Furthermore, decoupling the final heat exchanger network design from the energy and major equipment cost targets (such as compressors and turbines) ensures model reliability and robustness. This case study is formulated as a non-convex Mixed-Integer Non-Linear Programming (MINLP) problem, consisting of 2, 752 equations, 2, 065 variables, and 45 binary variables. It was solved to global optimality using the GUROBI solver [16] in 6.5 seconds using a personal computer (Intel(R) Core(TM) i7-10700 2.90GHz with 32 GB RAM)

ACKNOWLEDGEMENTS

The authors gratefully acknowledge financial support from the «Ministerio de Ciencia, Innovación y Universidades» from Spain under the project PID2024-155232NB-I00 -Net-0-ChemI-.

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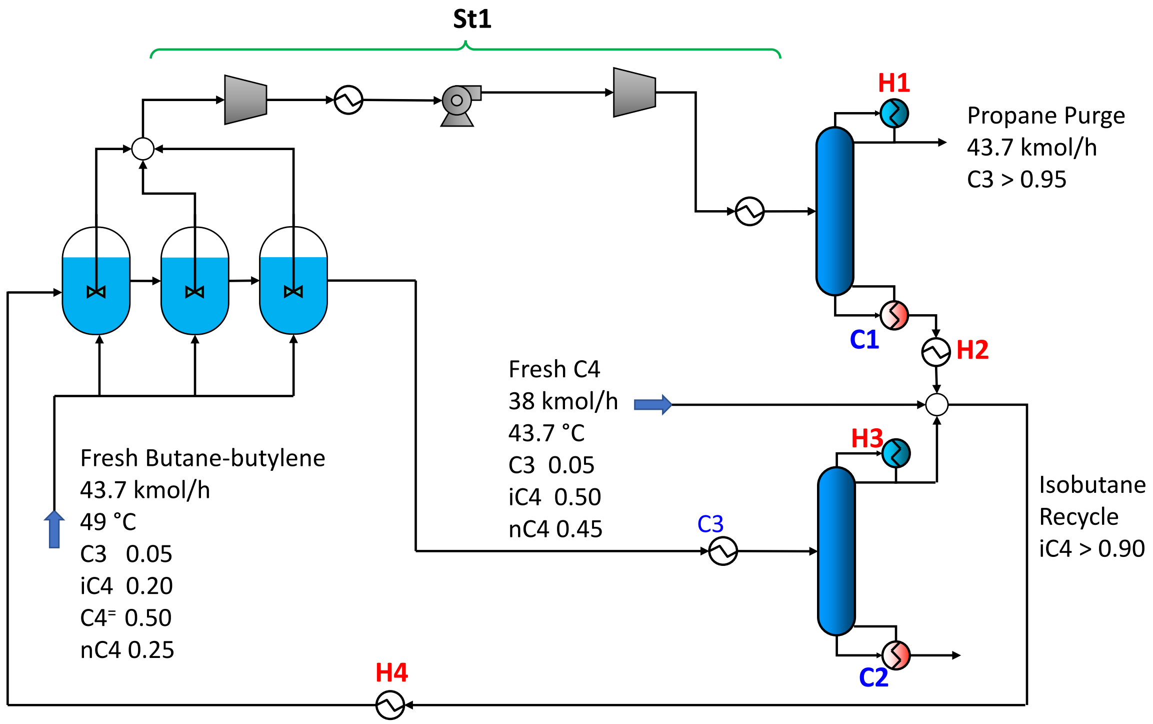

Figure 2. Flowsheet scheme indicating the streams that form part of the work and heat exchanger network

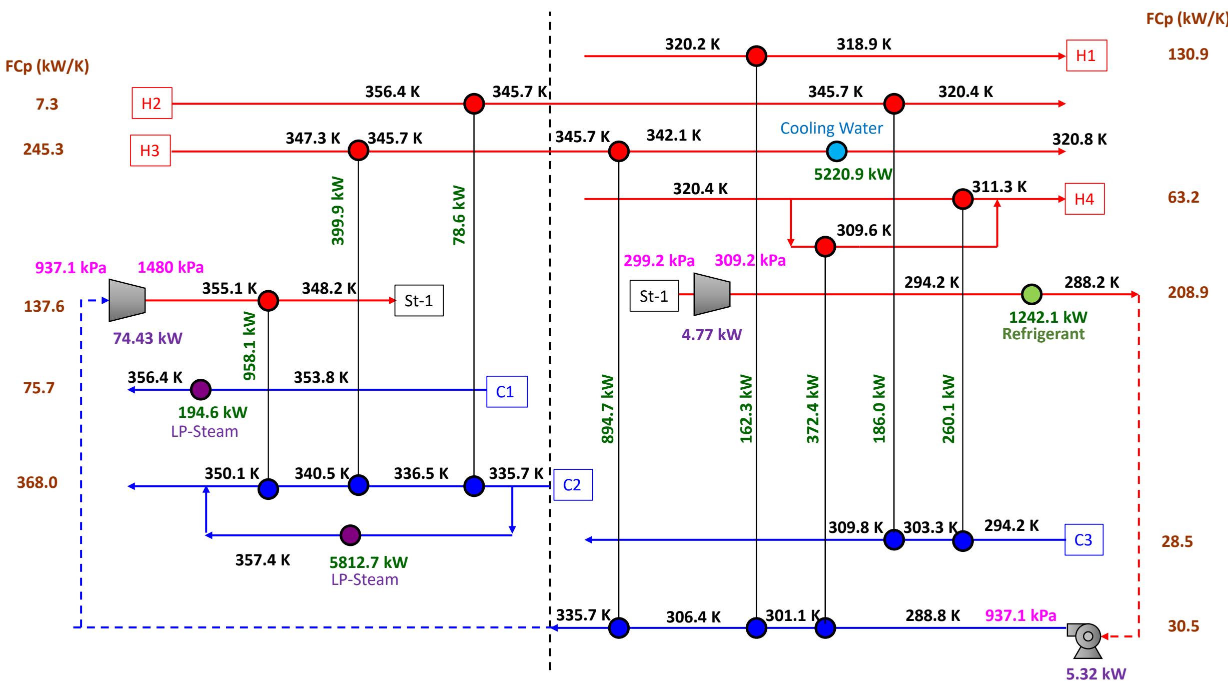

Figure 3: Heat exchanger network for the Case Study 1 optimal solution. Streams H1–H4 are hot process streams,

REFERENCES

1. Yu H, Fu C, Gundersen T. Work exchange networks (wens) and work and heat exchange networks (whens): a review of the current state of the art. Ind. Eng. Chem. Res. 59:507-525 (2019). https://doi.org/10.1021/acs.iecr.9b04932
2. Townsend DW, Linnhoff B. Heat and Power Networks in Process Design Part I: Criteria for Placement of Heat Engines and Heat Pumps in Process Networks. AIChE J 1983;29:742–7.

3. Colmenares TR, Seider WD. Heat and power integration of chemical processes. AIChE Journal 33:898-915 (2004). https://doi.org/10.1002/aic.690330604
4. Huang YL, Fan LT. Analysis of a work exchanger network. Ind. Eng. Chem. Res. 35:3528-3538 (1996). https://doi.org/10.1021/ie9507383
5. Aspelund A, Berstad DO, Gundersen T. An extended pinch analysis and design procedure utilizing pressure based exergy for subambient cooling. Applied Thermal Engineering 27:2633-2649 (2007). https://doi.org/10.1016/j.applthermaleng.2007.04.017
6. Onishi VC, Ravagnani MASS, Caballero JA. Simultaneous synthesis of heat exchanger networks with pressure recovery: optimal integration between heat and work. AIChE Journal 60:893-908 (2013). https://doi.org/10.1002/aic.14314
7. Fu C, Gundersen T. Integrating compressors into heat exchanger networks above ambient temperature. AIChE Journal 61:3770-3785 (2015). https://doi.org/10.1002/aic.15045
8. Fu C, Gundersen T. Integrating expanders into heat exchanger networks above ambient temperature. AIChE Journal 61:3404-3422 (2015). https://doi.org/10.1002/aic.14968
9. Fu C, Gundersen T. Sub-ambient heat exchanger network design including compressors. Chemical Engineering Science 137:631-645 (2015). https://doi.org/10.1016/j.ces.2015.07.022
10. Fu C, Gundersen T. Sub-ambient heat exchanger network design including expanders. Chemical Engineering Science 138:712-729 (2015). https://doi.org/10.1016/j.ces.2015.09.010
11. Nair SK, Nagesh Rao H, Karimi IA. Framework for work?heat exchange network synthesis (WHENS). AIChE Journal 64:2472-2485 (2018). https://doi.org/10.1002/aic.16129
12. Quirante N, Caballero JA, Grossmann IE. A novel disjunctive model for the simultaneous optimization and heat integration. Computers & Chemical Engineering 96:149-168 (2017). https://doi.org/10.1016/j.compchemeng.2016.10.002
13. Onishi VC, Quirante N, Ravagnani MASS, Caballero JA. Optimal synthesis of work and heat exchangers networks considering unclassified process streams at sub and above-ambient conditions. Applied Energy 224:567-581 (2018). https://doi.org/10.1016/j.apenergy.2018.05.006
14. Luyben WL. Principles and case studies of simultaneous design. Wiley (2011). https://doi.org/10.1002/9781118001653
15. Turton R, Bailei RC, Whiting WB, Shaeiwitz, J. A., & Bhattacharyya D. Analysis, Synthesis and Design of Chemical Processes. 5th editio. Upper Saddle River, NJ. USA.: Pearson Education, Inc.; 2018.
16. Gurobi Optimization L. Gurobi Optimizer Reference Manual 2025.