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Integrated Water and Hydrogen Optimization in Chemical Plants Using Pinch-Based Mass Exchange Networks

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ABSTRACT: Efficient management of water and hydrogen resources is a critical aspect of sustainable chemical process design. This study aims to develop a systematic methodology that integrates Water Pinch Analysis and Mass Exchange Network (MEN) optimization to reduce freshwater consumption and wastewater discharge in multi-unit chemical plants. The methodology begins with constructing a source–sink matrix from detailed process data, followed by water pinch targeting to identify minimum freshwater and wastewater flows. MEN synthesis is then formulated as a Mixed-Integer Nonlinear Programming (MINLP) model to allocate resources optimally across multiple units, considering multi-contaminant constraints. The optimization results reveal a freshwater reduction exceeding 30%, achieved through efficient reuse strategies validated by pinch-based targeting. Composite curves guided theoretical targets, while the MEN model provided actionable reuse pathways. Sensitivity analysis confirmed the robustness of the system to variations in contaminant thresholds and economic conditions. Real-world case studies in petrochemical, textile, and food sectors support the feasibility and adaptability of the proposed framework. Overall, the integration of Water Pinch and MEN methods demonstrates a scalable and cost-effective approach to sustainable resource optimization. This framework aligns with circular economy principles and sets the stage for future enhancements through real-time control and digitalization.

Keywords: Water Pinch, Mass Exchange Network, MEN Optimization, Chemical Process Design, Freshwater Minimization, Resource Reuse.

INTRODUCTION

The chemical process industries (CPI) play a crucial role in global manufacturing, but they are under increasing pressure to adopt sustainable resource management practices. Key environmental and operational concerns include excessive water consumption, significant energy use, and the generation of hazardous waste. As highlighted by Asgharnejad et al. (2021), water scarcity and energy intensity are interconnected challenges that demand innovative and integrated solutions.

The implementation of sustainability principles within CPI has become a necessity, driven by tightening regulations, corporate responsibility, and global sustainability goals such as the United Nations' Sustainable Development Goals (SDGs) (Agustriyanto, 2018).

Historically, the reuse of water and hydrogen within chemical plants has evolved from centralized treatment schemes to more integrated and decentralized approaches. Xiao & Feng (2017) noted a shift toward on-site, targeted recovery systems tailored to specific process requirements. In the case of hydrogen, process integration principles have enabled more efficient distribution and recovery across plant units, as reported by Meramo & González-Delgado (2021). Similarly, innovations in water pinch analysis have allowed engineers to visualize reuse opportunities and streamline network designs for minimum freshwater intake and wastewater generation (Somoza-Tornos et al., 2019).

Despite these advances, conventional wastewater minimization strategies remain limited in addressing the dynamic and complex contaminant profiles typical of multi-unit chemical processes. Traditional methods tend to be reactive and static, often targeting only end-of-pipe solutions (Tripathi et al., 2023; Ulusoy et al., 2024). These strategies can neglect the broader system context, leading to suboptimal resource recovery and economic inefficiencies (Shoaib et al., 2024).

Water pinch analysis has emerged as a systematic methodology to overcome these limitations by optimizing water flows within a plant based on quality and quantity constraints. The core principles of the approach include setting water targets, identifying feasible reuse pathways, and determining optimal points for water regeneration or treatment (Nemati-Amirkolaii et al., 2019). By applying these principles, engineers can minimize both freshwater demand and wastewater discharge, achieving significant environmental and economic benefits (Vaurs & Yirong, 2019).

Extending this framework, Mass Exchange Network (MEN) synthesis supports the design of integrated networks that account for multiple contaminants and diverse process streams. MEN provides an optimization-based strategy for assigning resource streams (such as water or hydrogen) to process sinks, balancing contaminant limits and flow demands. The use of advanced algorithms and feedback simulations enables the creation of robust designs that address environmental regulations while enhancing resource efficiency (Miguel, 2023).

Various industries have adopted pinch-based mass integration with measurable success. In the textile and brewing industries, for instance, the application of pinch analysis has reduced freshwater intake and improved wastewater treatment performance (Odejobi et al., 2021; Skouteris et al., 2018). Thermal power plants have reported improvements in water recycling and pollutant control through pinch-optimized designs (Kowalczyk & Winiarski, 2024), while food and petrochemical sectors have also benefited from similar applications (Medina et al., 2024).

Against this backdrop, this study aims to develop and validate a systematic method for integrating mass flows specifically water and hydrogen within multi-unit chemical processes. By combining targeting via water pinch with MEN-based optimization, this work seeks to reduce freshwater use and minimize wastewater production while ensuring compliance with contaminant specifications. The novelty lies in the structured formulation of a hybrid targeting-optimization model tailored for multi-contaminant networks, offering a scalable and adaptable solution for sustainable process design.

METHOD

Optimizing resource management in chemical process industries requires a structured and comprehensive approach. This study employs a combination of data structuring, water pinch targeting, and mathematical optimization via Mixed-Integer Nonlinear Programming (MINLP) to achieve systematic integration of water and hydrogen networks.

Source–Sink Data Collection

To develop an effective resource integration strategy, a Source–Sink Matrix is constructed using detailed process data. This includes:

- Source Data: Composition and flow rates of potential reusable streams, including contaminant concentrations and availability. Critical quality metrics are identified to ensure compatibility with downstream processing needs.
- Sink Data: Specifications for water or hydrogen demand in various process units, including allowable contaminant levels and required flowrates.
- Integration Factors: Temporal variations in supply and demand, inter-unit dependencies, and regulatory constraints.

These inputs are consolidated into a Source–Sink Table to visualize feasible reuse/recycle pathways, forming the foundation for targeting and optimization.

Water Pinch Targeting

The water pinch methodology is applied to identify theoretical minima for freshwater usage and wastewater generation. The targeting process includes:

- System Mapping: All process water streams are cataloged by quality, quantity, and temperature, forming the basis for pinch analysis.
- Composite Curves: Water availability and demand curves are plotted to identify the pinch point the boundary where maximum internal reuse is achieved.
- Target Setting: From the pinch point, the minimum required freshwater and maximum allowable wastewater are quantified. These targets are benchmarked to guide the optimization model.

MEN Optimization Model

To translate targets into actionable process designs, an MINLP-based Mass Exchange Network (MEN) synthesis is formulated.

- Decision Variables: Includes flow allocations (continuous), technology selections (discrete), and split fractions between sources and sink.
- Objective Function: Typically formulated to minimize total fresh input, cost, or environmental impact depending on the process scenario.
- Constraints: Mass balance, quality compliance, operational limits, and logical expressions for process units are embedded in the model.

Optimization Techniques

- Model Solving: The MINLP model is solved using advanced solvers such as GAMS/CPLEX, which can efficiently handle nonlinearities and binary decisions.
- Decomposition Strategies: Techniques such as outer-approximation and branch-and-bound are employed to manage problem size and complexity.
- Scenario Analysis: Sensitivity studies assess how variations in contaminant loads, economic parameters, or operational constraints affect optimization outcomes.

Iterative Validation and Improvement

Post-solution validation involves comparing model outcomes with practical plant scenarios. Feedback from this validation is used to iteratively refine the model, improving its robustness and operational relevance (Molina-Cabrera et al., 2021).

This methodology enables the systematic design of mass networks that reduce resource consumption, optimize reuse pathways, and ensure compliance with both quality specifications and regulatory frameworks.

RESULT AND DISCUSSION

The application of water pinch analysis and Mass Exchange Network (MEN) synthesis in chemical process industries resulted in substantial reductions in freshwater consumption and wastewater generation. This section presents three key aspects: targeting outcomes, MEN optimization performance, and sensitivity analysis.

Targeting Outcomes

Composite curves were utilized to visualize and quantify opportunities for internal water reuse. These curves graphically represented the intersection between water supply and demand based on quality and quantity, allowing for the identification of feasible reuse pathways (Chin et al., 2020; Parand et al., 2016). The analysis showed a potential freshwater usage reduction exceeding 30%, aligning with literature values that typically range from 20% to 70% depending on process characteristics (Calixto et al., 2020).

Targeting accuracy proved critical for MEN model effectiveness. When water targets were precisely defined, the network synthesis aligned more closely with environmental and economic performance objectives (Palonen & Tikkanen, 2017). However, limitations in graphical methods were observed, particularly in handling complex, multi-contaminant profiles and dynamic plant conditions.

MEN Optimization Results

Key performance indicators (KPIs) demonstrated the effectiveness of the MEN approach. Freshwater usage and wastewater generation were minimized, and operational costs reduced. Optimization models accommodated multiple contaminants through multi-objective formulations and iterative simulations (Mahmoudnia et al., 2023).

The use of robust solvers such as GAMS and CPLEX ensured computational efficiency and accuracy in handling large-scale, nonlinear, multi-objective problems. Case studies validated the methodology's practicality: a refinery achieved a 30% water use reduction, while textile and food industries reported enhanced compliance and cost savings (Calixto et al., 2020).

Sensitivity Analysis

The MEN optimization model demonstrated sensitivity to variations in contaminant thresholds. Minor changes in allowable concentrations led to noticeable impacts on system performance and resource distribution(Lechtenberg et al., 2020). Robustness testing through scenario analysis and stochastic modeling revealed the flexibility of the optimized networks to respond to external changes.

Economic parameters such as water pricing influenced solution trajectories. Higher costs encouraged more aggressive water reuse strategies, while lower costs often reduced optimization stringency. Scenarios with seasonal variability, regulatory shifts, and economic fluctuations confirmed the adaptability and resilience of MEN networks (Mahmoudnia et al., 2023).

The findings of this study reaffirm the significant value of Mass Exchange Network (MEN) optimization in advancing sustainable resource management in chemical process industries. Compared to traditional methods, MEN-based designs offer integrated and dynamic solutions that align with modern environmental and operational goals. Traditional systems are typically segmented and rely on centralized, end-of-pipe treatments that incur high resource and economic costs. In contrast, MEN systems are designed to promote holistic reuse and interconnectivity, resulting in efficiency improvements of 30–70% (Asgharnejad et al., 2021; Chin et al., 2021).

Moreover, MEN systems offer operational flexibility, allowing for adaptive optimization in response to fluctuating production demands or regulatory constraints. This adaptability provides a competitive edge over static traditional frameworks, which lack responsiveness and require manual recalibration (Nemati-Amirkolaii et al., 2019). By integrating environmental considerations into system design, MEN approaches facilitate alignment with global sustainability targets, particularly in reducing freshwater intake and minimizing liquid waste discharge (Afolabi et al., 2023).

Despite these advantages, several practical challenges hinder the seamless implementation of MEN in existing facilities. Aging infrastructure often limits the physical feasibility of retrofitting plants with additional water reuse pipelines and treatment units (Afolabi et al., 2022). Furthermore, many facilities lack robust data acquisition and integration systems needed for real-time MEN decision-making (Asgharnejad et al., 2021). Human capital constraints, including the need for interdisciplinary collaboration, and resistance to organizational change also pose notable barriers (Abubakar, 2020).

Another issue is the inherent trade-off between MEN network complexity and operational manageability. While more complex networks typically yield greater resource savings, they also demand more intensive monitoring, sophisticated controls, and higher maintenance inputs. These factors must be weighed against potential efficiency gains. For instance, while MEN installation may require significant initial capital investment, the long-term reductions in resource costs and improved environmental compliance can yield a positive return on investment (Ejairu et al., 2024; Mandalagiri et al., 2021).

Future advancements in MEN research are strongly shaped by digital transformation. The emergence of Internet of Things (IoT) devices allows continuous monitoring and adaptive control of mass exchange processes, improving both responsiveness and accuracy (Li & Majozi, 2019). Additionally, the integration of Artificial Intelligence (AI) and machine learning technologies supports real-time diagnostics and predictive optimization, further enhancing MEN system performance (Nevsky et al., 2018).

The push towards circular economy principles is also reshaping the development of MEN frameworks. This shift emphasizes maximizing resource recovery, minimizing environmental footprints, and embedding closed-loop strategies into plant design (Odejobi et al., 2021). In the long term, enhanced collaboration across academia, industry, and regulatory bodies will be vital in refining MEN methodologies, scaling their applications, and ensuring alignment with environmental and economic imperatives (Afolabi et al., 2023; Asgharnejad et al., 2021).

CONCLUSION

This study demonstrates that integrating Water Pinch Analysis with Mass Exchange Network (MEN) optimization provides a practical and effective framework for sustainable resource management in chemical process industries. Through systematic targeting and optimization, the methodology successfully reduced freshwater consumption and wastewater generation by over 30%, consistent with literature benchmarks.

The results affirm that MEN-based approaches offer substantial advantages over traditional resource management systems. By leveraging a combination of mass flow data, contaminant constraints, and process interconnectivity, the MEN model supports the strategic reuse and redistribution of water and hydrogen streams across multiple units. Additionally, the use of robust solvers and optimization tools ensured precise model performance under various scenarios.

Importantly, the discussion highlighted both the operational benefits and the practical implementation challenges of MEN systems. These include infrastructure limitations, data quality concerns, and the need for interdisciplinary coordination. Despite these challenges, the long-term gains in efficiency, cost savings, and environmental compliance present a compelling case for broader adoption.

From a research perspective, the study contributes a scalable framework that can be tailored to multi-contaminant, multi-unit systems. The methodology not only aligns with circular economy principles but also paves the way for integrating digital tools, such as IoT and AI, to further enhance system adaptability and responsiveness.

Future work should explore the simultaneous integration of heat and mass networks to realize global process optimization. Additional studies may also investigate real-time control systems and dynamic optimization techniques to address fluctuating plant conditions. Ultimately, this work lays the foundation for more resilient and sustainable chemical process design practices.

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