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DynHeat: Heat Exchanger Network Design for Batch Processes via Dynamic Optimization

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Abstract

Heat integration can reduce the consumption of external utilities in batch processes. Batch processes often include process steps with dynamic temperature progression, such as heating in vessels. During heat integration between those process steps, the temperature difference decreases over time. Exploiting the thermodynamic potential for heat integration can, therefore, lead to long process durations. Hence, there is a trade-off between the total cost of heat integration and the process duration. A method is missing to map this trade-off while considering the dynamic temperature progression. We introduce the DynHeat optimization method for heat exchanger network design in dynamic batch processes based on dynamic optimization. We apply the DynHeat method to a case study and perform a multi-objective optimization regarding the process duration and the total cost. We find that the DynHeat method can propose a suitable heat exchanger network design and operation mode for the regarded case study.
Keywords: Energy Efficiency, Heat Integration, Pinch Method, Logarithmic Mean Temperature Difference, Dynamic Processes

1. Introduction: Heat Integration in Batch Processes

Meeting thermal energy demands in industrial processes by external utilities is economically and environmentally expensive. Heat integration can reduce the consumption of external utilities by reusing waste heat. For heat integration, a heat exchanger network needs to be built. To obtain cost-optimal heat exchanger networks, the total cost should be considered, comprising operational costs for utility consumption and investment costs for heat-exchangers.

Common existing approaches for heat exchanger network design, based on the Pinch Method (Linnhoff and Flower, 1978) or the superstructure model by Yee and Grossmann (1990) and most of their extensions, reviewed by Klemeš and Kravanja (2013), assume stationary process streams. In practice, many industries work with instationary batch processes. In batch processes, the products are often cooled down or heated up in vessels, which leads to temperatures changing over time. When using heat integration in such processes, the transferred heat between two products decreases over time as the temperature difference between those products decreases. Thus, exploiting the full thermodynamic potential for heat integration between two products leads to long process durations. Hence, heat integration in dynamic batch processes causes a trade-off between process duration and total cost for heat integration. This trade-off needs to be considered when designing heat exchanger networks for dynamic batch processes. A suitable method for heat exchanger network design for dynamic batch processes should, thus, represent the dynamic temperature profiles accurately to determine both the amount of integrated heat and the process duration.

In practice, the Pinch Method is commonly used for estimating the thermodynamic potential for heat integration of a process. The Pinch Method can be adapted to varying thermal demands by averaging the demands over time (time-average model) or by dividing the time horizon into several time slices (time-slice model) (Kemp and Lim, 2020). However, both approaches still assume temporary stationary process streams. Vaselenak et al. (1986) propose a heuristic method to handle different types of temperature progression of batch products in tanks in heat integration problems. Dowidat et al. (2014) extend the time-slice model to dynamic temperature progression by introducing additional time slices. However, both approaches do not explicitly design a heat exchanger network. In Dowidat et al. (2016), the authors introduce a match ranking matrix for the design of economically efficient heat exchanger networks. However, the approach relies on heuristic rules instead of considering the actual costs. Furthermore, in all the approaches mentioned above, the timing of the processes needs to be known in advance, and the trade-off between process duration and total costs, is not taken into account. Castro et al. (2015) introduce an optimization model for combined heat integration and scheduling in order to optimize the makespan of the process. However, in their approach, matches between process streams can be derived but no design optimization is included.

In conclusion, no optimization method exists that can represent the trade-off between process duration and total cost for thermal energy supply in heat integrated dynamic batch processes. In this contribution, we bridge this gap by developing the DynHeat optimization method for heat exchanger network design of dynamic batch processes while taking the trade-off between total cost and the process duration into account.

2. The DynHeat Method

The aim of the DynHeat method is to design a heat exchanger network for dynamic batch processes while taking the trade-off between total cost, comprising operational costs and investment costs, and the process duration into account. In the corresponding DynHeat optimization model, we model products that either need to be heated or cooled in vessels. The thermal demands can be provided by external utilities or via heat integration. For heat integration, there is the option of building an external heat exchanger between every two vessels. A scheme of the DynHeat model is shown in *Figure 1*.

To address the trade-off between cost and duration, we perform a multi-objective optimization with the total cost C^{total} of one process run as one objective function and the process duration τ^{final} as the other objective function. The total cost C^{total} for one process run are composed of the investment cost for the heat exchangers and operational cost for external utility:

$$C^{total} = \left(\sum_{h \in H} (A_h^{cu} + A_h^{HI}) + \sum_{c \in C} (A_c^{hu} + A_c^{HI}) + \sum_{h \in H} \sum_{c \in C} A_{h,c}^{HE} \right) c^A + \sum_{h \in H} Q_h^{cu} \; c_h^{cu} + \sum_{c \in C} Q_c^{hu} \; c_c^{hu} \quad (1)$$

With the surface areas of the heat exchangers for hot utility (A_h^{cu}), cold utility (A_c^{hu}), hot product to heat transfer media (HTM) (A_h^{HI}) and cold product to HTM (A_c^{HI}) and the external heat exchanger ($A_{h,c}^{HE}$). The cost factor c^A refers to the specific investment costs for the heat exchanger surface areas scaled down to one process run. The operational costs comprise the amount of heat supplied by the cold utility Q_h^{cu} and hot utility $Q_c^{hu}$and the specific price for cold utility c^{cu} and hot utility c^{hu}.

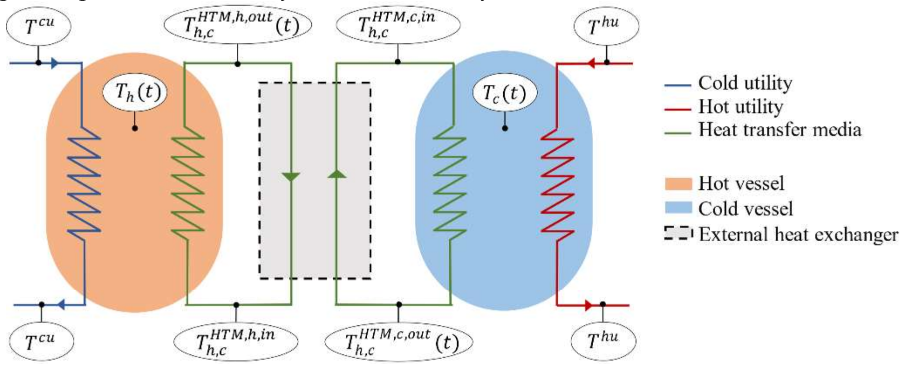

Figure 1: Exemplary scheme of the DynHeat model for one hot and one cold product. The left vessel (orange) contains the hot product of the temperature $T_h(t)$ which can be cooled down by cold utility of the temperature T^{cu} (dark blue). Analoguesly the cold product in the right vessel (light blue) of the temperature $T_c(t)$ can be heated up by hot utility (red) of the temperature T^{hu}. Both vessels can be connected by an external heat exchanger (grey) with heat transfer media (HTM) (green line). The temperature of the HTM at the inlet of the vessels $T_{h,c}^{HTM,h,in}$ and $T_{h,c}^{HTM,c,in}$, is constant.

In the DynHeat model, we make the following assumptions: The vessels are perfectly mixed, and no heat losses occur. The external heat exchangers are counter-flow heat exchangers. All heat capacities, heat transfer coefficients, and the temperature of the utilities are constant. The HTM is not allowed to function as a storage, i.e., the total integrated heat flow must be transferred from the hot product to the cold product immediately, and the temperature of the HTM at the inlets of the vessels $T_{h,c}^{HTM,c,in}$ and $T_{h,c}^{HTM,h,in}$ is constant. The HTM between a hot and a cold product has the same heat capacity rate on both sides of the external heat exchanger, i.e., the temperature difference along the external heat exchanger $(T_{h,c}^{HTM,h,in} - T_{h,c}^{HTM,h,in}(t)) = \left(T_{h,c}^{HTM,h,out}(t) - T_{h,c}^{HTM,c,in}\right)$ is constant along the heat exchanger surface area.

In the following, we describe the DynHeat model in detail. The most important equations are given for hot products that need cooling. The equivalent equations for cold products that need heating can be derived analogously.

The temperature profile $T_h(t)$ of a hot product h with the mass m_h and heat capacity $c_{p,h}$ changes due to heat transferred to cold utility $\dot{Q}_h^{cu}(t)$ or by heat integration with a cold product $\dot{Q}_{h,c}^{HI}(t)$:

$$\frac{dT_h(t)}{dt} = -\frac{\left(\sum_{c\in C}\dot{Q}_{h,c}^{HI}(t)\right) + \dot{Q}_h^{cu}(t)}{m_h \cdot c_{p,h}} \qquad \forall h \in H \qquad (2)$$

The heat flow from a hot product to the HTM $\dot{Q}_{h,c}^{HI}(t)$ is defined by

$$\dot{Q}_{h,c}^{HI}(t) = \dot{m}_{h,c}^{HTM}\, c_p^{HTM}\left(T_{h,c}^{HTM,h,out}(t) - T_{h,c}^{HTM,h,in}\right) \qquad \forall h \in H, \forall c \in C \qquad (3)$$

, where $\dot{m}_{h,c}^{HTM}$ is the given mass flow of the HTM between hot vessel h and cold vessel c and c_p^{HTM} is the given constant heat capacity of the HTM.

The temperature of the HTM at the outlet of the hot vessel $T_{hc}^{HTM,h,out}(t)$ is defined by the temperature progression along the heat exchanger between the hot product and the HTM (Glück, 2017):

$$T_{h,c}^{HTM,h,out}(t) = T_{h,c}^{HTM,h,in}(t) \cdot e^{-\frac{k\ A_{h,c}^{HTM,h}}{\dot{m}_{h,c}^{HTM}\ c_p^{HTM}}} + T_h(t) \cdot \left(1 - e^{-\frac{k\ A_{h,c}^{HTM,h}}{\dot{m}^{HTM}\ c_p^{HTM}}}\right) \qquad \forall h \in H, \forall c \in C \qquad (4)$$

, where $A_{h,c}^{HTM,h}$ is the surface area of the heat exchanger between the hot product and the HTM, and k is the constant heat transfer coefficient of the heat exchanger.

Finally, the required surface area of the external heat exchanger $A_{h,c}^{HE}$ can be derived by the transferred heat and the temperatures of the heat transfer medium by

$$\dot{Q}_{h,c}^{HI}(t) \geq k\ A_{h,c}^{HE}\ \Delta T_{h,c}^{HTM}(t) \qquad \forall h \in H, \forall c \in C \qquad (5)$$

, where the temperature difference $\Delta T_{h,c}^{HTM}(t)$ describes the temperature difference in the external heat exchanger. As in Verheyen and Zhang (2006), we assume that the biggest surface area needed at any time is installed and that all other operation modes can be realized by bypassing a part of the streams. The heat exchanger surface area for utility supply can be derived analogously. We assume a sequential process, meaning that external utilities are only used after heat integration is complete. Logical big-M constraints denote the beginning and end of utility supply and heat integration.

To solve the resulting dynamic-algebraic optimization problem, we discretize the time by orthogonal collocation on finite elements using pyomo.dae (Nicholson et al., 2018). Through the collocation, the discretized problem is a fully algebraic mixed-integer nonlinear optimization problem (MINLP) (Biegler, 2010).

3. Application to a Case Study

We apply the DynHeat method to a case study with one hot and one cold product. We adapt our process parameters to a milk pasteurization process, where fresh milk is first heated to a certain temperature and, afterwards, is cooled down to its final storing temperature. We assume that the heating of one batch and the cooling of another batch take place simultaneously. We adapt the process parameters from a case study in Fellows (2017) .

We compute the case study on an Intel(R) Xeon(R) CPU E5-1660 v4 with 3.30GHz running on Microsoft Windows Server 2016 Standard with kernel version 10.0.14393. We use python 3.7 as a modeling language. As a solver, we use baron version 20.4.14 (Kılınç and Sahinidis, 2018). We apply eight threads. The relative gap is set to 1E-8. For the collocation method, we choose seven finite elements and 3 collocation points per element. We set a limit of 1000 sec to the time horizon to facilitate the solution of the problem.

With the DynHeat model, we perform a multi-objective optimization of the given case study, minimizing the process duration and the total cost of one process run. Figure 2 (left) shows the resulting Pareto front for the selected case study. The Pareto front visualizes the trade-off between the total cost for one process run and the process duration.

In the left anchor point, the total cost is minimal. Heat integration takes place as long as possible, such that the smallest possible amount of utility is used. However, thereby the maximal allowed time horizon of 1000 sec is required. In contrast, the right anchor point shows the results for minimal process duration. For minimal process duration, the thermal demands are covered by utility only. By the increased use of external utility, the total cost increase by almost 60% compared to the minimal total cost. Accordingly, heat integration can significantly reduce the total cost in the regarded case study.

Furthermore, there is one solution point between the two anchor points, representing a compromise between process duration and total cost. Figure 2 (right) shows the temperature profiles and the heat flows for the compromise solution. The heat integration is stopped before the temperature of the hot and the cold product reach the same level. Instead, a temperature difference of $19.02\ K$ remains and utility is used to cover the remaining demands. This compromise increases the total cost only slightly, while reducing the process duration by almost $600\ sec$ compared to the left anchor point.
All in all, the Pareto front shows that heat integration can reduce the total cost significantly in the regarded case study. However, heat integration extends the process duration notably. Given this trade-off, the DynHeat method also offers solutions with a finite process duration that still significantly benefit from heat integration.

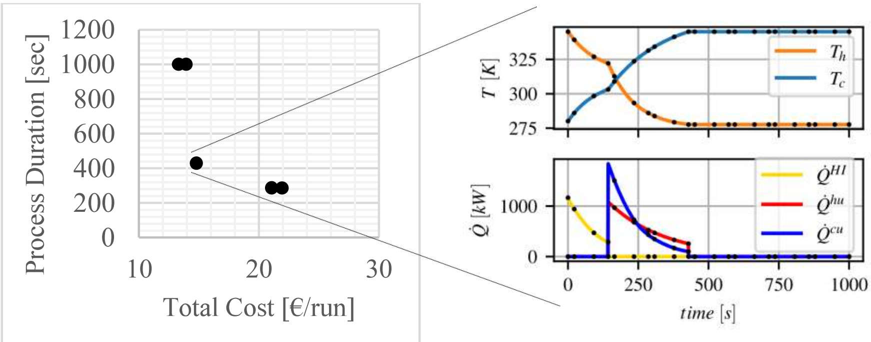

Figure 2: Left: Resulting Pareto front of the DynHeat method for the selected case study. Right: Process operation for one middle point on the Pareto front. The upper diagram shows the temperature progression of the hot product $T_h(t)$ (orange) and the cold product $T_c(t)$ (blue) over time. The lower diagram shows the corresponding heat flows (heat integration $\dot{Q}_{h,c}^{HI}(t)$ (yellow), cold utility $\dot{Q}_h^{cu}(t)$ (blue) and hot utility $\dot{Q}_c^{hu}(t)$ (red)).

While the orthogonal collocation in the DynHeat method allows for a more accurate representation of the dynamic temperature profiles than existing approaches, it still leads to some discretization errors. The dynamic profiles are not represented exactly but approximated by polynomials. In our case, the DynHeat method leads to a discretization error concerning the integrated heat of $1.1\ \%$. Thus, we conclude that the chosen settings are sufficient for accurate representation of the temperature profiles. Furthermore, due to the discretization, the process can only switch from heat integration to utility supply, and also finish the utility supply, at the boundaries of a finite element of the discretized time horizon. Consequently, the obtained solutions highly depend on the number of finite elements. The discretization, thus, restricts the solution space, but all solutions of the discretized problem are feasible to the original problem.
With the chosen settings, we find that the DynHeat model does not terminate to global optimality within the allowed computing time of $3000\ sec$ for all points on the pareto front. Thus, further research on the model complexity and solvability needs to be done. However, the results show that the DynHeat model can propose reasonable solutions for heat integration in batch processes while considering dynamic temperature changes.

4. Conclusion

In this contribution, we introduce the DynHeat method for heat exchanger network design in dynamic batch processes. We model the temperature dynamics of the batch process and discretize the problem by orthogonal collocation to a fully algebraic MINLP. To the best of our knowledge, the DynHeat method is the first optimization method that meets the trade-off between process duration and total cost for heat integration in dynamic batch processes while taking design decisions for heat exchangers into account. We find that the DynHeat method enables us to find solutions that offer a compromise between total cost and process duration.

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References

L.T. Biegler, 2010, Nonlinear programming. Society for Industrial and Applied Mathematics, Philadelphia, Pa.

P.M. Castro, B. Custódio, H.A. Matos, 2015, Optimal scheduling of single stage batch plants with direct heat integration, Comput Chem Eng, vol. 82, 172

C. Dowidat, M. Kalliski, G. Schembecker, C. Bramsiepe, 2016, Synthesis of batch heat exchanger networks utilizing a match ranking matrix, Appl Therm Eng, vol. 100, 78

C. Dowidat, K. Ulonska, C. Bramsiepe, G. Schembecker, 2014, Heat integration in batch processes including heat streams with time dependent temperature progression, Appl Therm Eng, vol. 70, 1, 321

P. Fellows, 2017, Food processing technology. Woodhead Publishing, Duxford, United Kingdom

B. Glück, 2017, Wärmeübertrager, Raumheizflächen, Behälteraufheizung, Verl. für Bauwesen, Berlin

I.C. Kemp, J.S. Lim, 2020, Pinch Analysis for Energy and Carbon Footprint Reduction: User Guide to Process Integration for the Efficient Use of Energy. Butterworth-Heinemann

M.R. Kılınç, N.V. Sahinidis, 2018, Exploiting integrality in the global optimization of mixed-integer nonlinear programming problems with BARON, Optimization Methods and Software, vol. 33, 3, 540

J.J. Klemeš, Z. Kravanja, 2013, Forty years of Heat Integration: Pinch Analysis (PA) and Mathematical Programming (MP), Curr Opin Chem Eng, vol. 2, 4, 461

B. Linnhoff, J.R. Flower, 1978, Synthesis of heat exchanger networks: I. Systematic generation of energy optimal networks, AIChE J, vol. 24, 4, 633

B. Nicholson, J.D. Siirola, J.-P. Watson, V.M. Zavala, L.T. Biegler, 2018, pyomo.dae: a modeling and automatic discretization framework for optimization with differential and algebraic equations, Math Prog Comp, vol. 10, 2, 187

J.A. Vaselenak, I.E. Grossmann, A.W. Westerberg, 1986, Heat integration in batch processing, Ind Eng Chem Process Des Dev, vol. 25, 2, 357

W. Verheyen, N. Zhang, 2006, Design of flexible heat exchanger network for multi-period operation, Chem Eng Sci, vol. 61, 23, 7730

T.F. Yee, I.E. Grossmann, 1990, Simultaneous optimization models for heat integration—II. Heat exchanger network synthesis, Comput Chem Eng, vol. 14, 10, 1165