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Heat Exchanger Networks Synthesis Considering Dynamic Flexibility

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Previous studies on steady-state flexible design have shown that flexibility is essential to design profitable HENs undergoing the disturbances. However, chemical plants are complex dynamic systems that need to be operated successfully throughout the time in the presence of disturbances. Under these circumstances, the previous work should be extended to make dynamic flexible network engineered well. Based on the variation ranges of stream output temperatures, this paper proposes a feasible method for heat exchanger networks synthesis (HENS) involving dynamic flexibility. And then the above results are further analysed by considering the integration of dynamic flexibility and advanced control designs. This study begins with discretization of uncertainties and then generalized critical points are identified by the deviations of output temperatures derived from the simulation results containing the previous samples. Finally, the temperature variation ranges are defined as control range to optimize the degree of over-synthesis which generally introduces a waste of heat exchanger area for implementing flexible design, and to be an attractive alternative considering the coupling between dynamic flexible synthesis and control design. A case is subsequently considered to analyse the feasibility of the above framework and the significance of the proposed integration problem.

1. Introduction

Heat exchanger network synthesis (HENS) is still an active research since it largely determines the optimal and safe operation under various conditions. However, either profitable heat exchanger networks (HENs) or conventional HENS method has been generally performed following a fixed operation condition. Once the uncertainties have deviations from these nominal values, the practical economy and even feasibility will fail to be maintained. It is important to develop flexible HENS method for which the gap to practical process is minimal.

In the present safety-oriented chemical process system, considering dynamic performance features either significant importance or more rigorous since the practical process cannot be adequately characterised by the flexibility index, e.g. Shi and You (2015) considered robust and dynamic optimisation for continuous processes under uncertainty. Dimitriadis and Pistikopoulos (1995) introduced dynamic models as the model constraints and then proposed a dynamic flexibility index for dynamic flexibility analysis. Subsequently, the above work was discussed extensively by several other groups. Adi and Chang (2013) involved the disturbances' cumulative effects. Zhou and Li (2009) considered the initial conditions of the uncertainties. However, their computation burden and the intimate relationship with control strategy introduce limitation to the development. Besides, the aforementioned flexibility problems are merely employed to evaluate the capability which can withstand the time-varied disturbances. Therefore, the synthesis problem of flexible HENs is raised subsequently to achieve economic and flexible optimization objectives. However, contrast to the flexible design based on steady-state, dynamic flexible design fails to receive considerable attention, which results from greater computation burden and the similarity with the conventional integration of synthesis and control designs. Nevertheless, it still can be engineered well rather than severe dependency of this integration problem. Moreover, the appropriate overdesign resulting from the considerations of dynamic factors in the flexible synthesis design and the coupling relation of dynamic flexible and control designs can give sufficient

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degree of freedom and then circumvent expensive control cost. Hence, it is desired to incorporate dynamic flexible and advanced control design as a new integration problem.

The objective of this paper is to present a dynamic flexible design methodology that gives appropriate oversynthesis degree in terms of integration of dynamic flexible HENS and advanced control designs. The key idea is to determine the dynamic flexibility index instead the deviations from nominal values of stream output temperatures. And then the generalized critical operating points corresponding to the time-varied disturbances are identified by the maximum temperature deviations. In the context of the proposed integration problem, this developed method is an attractive alternative circumvent demand significant efforts from the control system.

2. Dynamic Flexible Design Methodology

The conventional integration is an effective method to handle the time-dependent realization in the disturbances. Similarly, dynamic flexible design can also handle the disturbances and the more important to it to be employed to find the trade-off between the over-synthesis degree and control quality, i.e. design cost and control cost. This method is developed through these trade-offs, which are derived by stream output temperature variation ranges.

Dynamic flexible design differs from steady-state flexible design in the sense that the dynamic models are considered as constraint and a series of time-varied disturbances are involved. But in spite of this difference, different flexible design can still bring about different degree of over-synthesis. Hence, this degree can be employed to measure the influence of flexible design on the profitable HENs. In this paper, variation range of stream output temperature is defined to represent the aforementioned degree in the premise of ensuring heat balance. This range is derived by the deviation from nominal value of stream output temperature. The feature to be noted is that greater range implies a loss associated with keeping the temperature around its set point. Besides, this range also has intimate relationship with either control cost or control quality. Therefore, the variation range of stream output temperature with regard to over-synthesis degree can be employed to effectively analyse the trade-off among design cost, control cost and control quality in the context of the proposed integration problem.

2.1 Process Disturbances

Previous flexible design and integration studies both assumed that there were time-independent stochastic disturbances or time-varied disturbances follow a certain function, e.g. a series of step changes. However, these two types both need to be considered to comprehensively construct the condition of multiple perturbations which exists in the real industrial world generally. Time-varied and stochastic disturbances need to be introduced in the dynamic flexible design. Bahakim and Ricardez-Sandoval (2014) suggested that this practical variability could follow a user-defined probability distribution function:

(1)

$$D_{S}(t) = \{D_{S} \mid D_{S} \sim \mathsf{PDF}(\alpha_{S})\}$$

Where D_s is the *s*th disturbance and α_s is the *s*th disturbance's parameter of the probability disturbance function PDF. Description Eq(1) represents that the disturbances are stochastic and the selection of PDF denoting this performance needs to be assigned by the user. Despite of the dynamic or time-dependent performance, the conventional PDF is suitable to describe the stochastic characteristic with respect to variability in the plant. However, the value at any time *t* cannot be specified. Bahakim and Ricardez-Sandoval (2014) also suggested that the stochastic disturbances' time-dependence could be represented by:

$$D_{\mathcal{S}}(t) = \sum_{q=1}^{q} D_{\mathcal{S}}(q)$$
(2)

Where *q* is sampling period and time $t = q \cdot \Delta t$. Δt is sampling interval and this relationship exists still in the ultimate time. Although this formulation's significance can be known to provide more appropriate description of variability, it fails to be involved in the design problem resulting from the demands of small interval and period. In order to simplify the dynamic flexible design problem, the disturbance's time-dependence can be obtained by:

$$D_{\mathcal{S}}(t) = \{\Delta t, D_{\mathcal{S}}(\Delta t)\}$$
(3)

The description (3) represents that the sth disturbance corresponds to the certain discrete time. The stochastic sampling in present method is selected to use a generalized random number generated function, i.e. the combination of Matlab internal random and time functions is employed to describe the dynamic stochastic variability. However, this simplified method involves only the specific sampling and time intervals. And then the generalized critical operating points, which are defined to have the similar significance with critical operating

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points and also indicate the limitation of dynamic flexibility on HENs, cannot denote the actual values. The network configurations can be comprehensively contained only if the PDF can introduce sufficiently wide range of probability distribution or the sampling and time intervals are small enough. This part will be studied in the future work.

2.2 Dynamic flexibility and generalized critical operating points

The steady-state flexibility analysis method can find flexibility index and the corresponding critical operating points simultaneously. Based on these operating points, the network configuration can be retrofitted and then the flexible network can be obtained. Although the dynamic flexibility analysis methods are generally developed on the basis of the steady-state flexibility analysis method, the generalized critical operating points. The traditional dynamic flexibility index considers maximum variation range of the uncertainties as the objective, i.e. the maximum feasible hyper-rectangle. But the usage of the dynamic and stochastic uncertainties leads to the difference between the conventional method and this work. This work proposes an attractive alternative to obtain the generalized critical operating points in the objective of maximum dynamic flexibility.

The work of generalized critical operating points begins with the construction of dynamic flexibility. It essentially belongs to the dynamic optimization problem as it contains dynamic models and mixed integer nonlinear program (MINLP). Dimitriadis and Pistikopoulos (1995) suggested either full discretization algorithms or control parameterization algorithms to calculate this dynamic optimization problem. Since the former method fails to handle the large-scale problem, this work uses the latter method and then a Matlab optimal control package (DYNOPT) is employed to calculate. Besides, the rigorous mathematical model of the conventional dynamic flexibility index is computationally intensive or prohibitive. Conversely, considering variation range of stream output temperature as either objective or dynamic flexibility of this developed method can lighten the calculation burden and also construct the coupling relation of flexible synthesis and control designs in subsequent integration problem. Therefore, the objective can be retrofitted as follows:

$$\min_{\boldsymbol{U}(\boldsymbol{t}),\boldsymbol{\rho}} \sum_{i} \left| \mathcal{T}_{\text{Hout},i}(\boldsymbol{t}_{f}) - \mathcal{T}_{\text{Hout},i}^{\mathsf{N}} \right| + \sum_{j} \left| \mathcal{T}_{\text{Cout},j}(\boldsymbol{t}_{f}) - \mathcal{T}_{\text{Cout},j}^{\mathsf{N}} \right|$$
(4)

Where T_{Hout} and T_{Cout} are the output temperatures of hot and cold streams respectively. T^{N} denotes the nominal value. *u* is manipulation variable (MV) with the purpose of finding the optimum objective and either the bypass fraction or utility consumption are generally selected. *p* involves the stochastic disturbance in last section. The subscript *i* and *j* represent the hot and cold stream respectively. The description (4) denotes the summation with respect to the variation ranges of the output temperatures. The noted feature is that minimum deviation from nominal value introduces preferable control quality and demands profitable efforts from the control system.

After that, the generalized critical operating points are defined as the points having maximum deviation from nominal value, which can be described as following:

$$\delta = \{ \max_{u(t), p} \xi_{t, S} \}$$
(5)

Where δ is the generalized critical operating point and consists of maximum of *i+j* elements. ξ is the deviation from nominal value of the output temperature, which is based on the results of the above dynamic optimization problem. The significance of description (5) is to identify the generalized critical points and each point denotes the corresponding discrete time and stochastic disturbance. This sequential method for calculation of dynamic flexibility and the identification of generalized critical operating point can effectively avoid from intensive or prohibitive computation.

2.3 HENs optimization for dynamic flexibility

For steady-state flexible synthesis design, the synchronous method is hard to be performed with this rigorous mathematical model or implemented with greater computation burden. Similarly, dynamic flexible design also fails to be implemented on account of the existence of discrete time. This work divides the dynamic flexible design problem into a series of steady-state flexible design and then these multiple configurations are consecutively optimized. Another difference with steady-state flexible design is that the evaluations from flexibility index are neglected. The sufficient heat exchange duty making stream output temperatures around their set points is employed instead.

Objective: the retrofitted total annual cost

min $TAC = OP^{ex} + CAP^{ex} + OP^{req} + CAP^{req}$

Where *OP* and *CAP* denote operating cost and capital cost respectively. The superscript ex and req are existed and purchased heat units. The feature to be noted is that the objective suggests fewer purchased heat units and retrofits existing heat units. This can bring about profitable configuration and sufficient degree of freedom on following optimizations.

Subject to:

The method employed in HENS for the previous work is based on the non-split two-stage superstructure involving all the possible bypasses. Therefore, part of the model for this work is the same, e.g. the heat balance in the stages. To facilitate the description, the stage, heat balances etc. are not contained in the following descriptions. Moreover, this method does not imply that it is only applicable to the HENs obtained by this superstructure. The mentioned superstructure is employed for illustrating the usefulness of the proposed method while it cannot be computationally intensive or prohibitive.

$$T_{\text{Hout},i} \leq T_{\text{Hout},i}^{\text{N}} + T_{\text{Hout},i}^{\text{N}} \cdot \varphi_{\text{H},i}$$

$$T_{\text{Hout},i} \geq T_{\text{Hout},i}^{\text{N}} - T_{\text{Hout},i}^{\text{N}} \cdot \varphi_{\text{H},i}$$
(8)

Where φ is defined as control range of stream output temperature which is employed to adjust the degree of over-synthesis and also introduce degree of freedom for sufficient heat exchange duty.

$$\sum_{n_{HE}} q_{\text{HE},ijk}^{tm} \ge \sum_{n_{HE}} q_{\text{HE},ijk}^{tm-1}, \quad (q_{\text{HE},ijk}^{tm-1} = q_{\text{HE},ijk}^{\text{N}}, tm = 1)$$
(9)

Where q_{HE} and n_{HE} are heat load and the number of heat exchangers respectively. *tm* is discrete time identified for the generalized critical operating point. The above represents the relationship between the network configurations of the adjacent times. It makes these network structures corresponding to time associate with each other. All the generalized critical operating points are arranged in the sequence of time and then the heat load of network in the former time outweighs that of the latter time, i.e. the network configuration of the former time is employed to evaluate that of the latter time. When the heat exchange duty of network is greater and the control ranges of the output temperatures are held, the dynamic flexibility design for this time is performed. But the monotonicity of heat exchange duty variation in the sequential time cannot be ensured, and then this will bring about the certain increase on the over-synthesis degree and also design cost. The consistency of heat exchange duty and time variation directions will be studied in the future.

$$\xi_{tm+1}^{ne} = A \cdot \xi_{tm}^{ex} + B \cdot \Delta u_{tm}^{ex} + C \cdot \Delta u_{tm}^{ne} \tag{10}$$

Where ξ_{tm+1}^{ne} is the temperature deviation of the optimized configuration in the tm+1 time. Similarly, ξ_{tm+1}^{ex} is

that of the existing structure in the *tm* time. *A* is the configuration coefficient, which denotes the relationship between the temperature deviations of the optimized and existing structures. *B* and *C* are control action coefficient and control optimization variable, which represents the influence of control action of the existing structure (*tm-1* time) on the optimized configuration and the control action of optimized configuration (*tm+1* time). Δu is the MV's variation resulting from keeping the output temperature around its set point. The situation which this paper does not involve the control design problem implies *C* can be equal to the specific constant. The noted feature is that since the relationship among *A*, *B* and *C* fails to be described, it needs to be defined by a series of inequality which are developed by the comparisons between the temperature variations of the adjacent times.

Besides, this model also contains the constraints of binary variables involving the existence of purchased and existed heat units, the heat transfer area, etc.



Figure 1a: Existing heat exchanger network with variables and data.

Figure 1b: Plot for the samples of operation uncertainty.

Figure 1c: Results of the dynamic optimization problem.

3. Case study

An example is given in this section to illustrate the proposed method. The models of network configuration optimization are formulated in GAMS and solved on an Intel Core 3.60 GHz machine with 3.46 GB memory. The solver BARON is employed to solve the MINLP problem. The generating of discrete sample, dynamic optimization problem and close-loop simulations are both performed in Matlab.

This case involved two hot streams and two cold streams as described by Grossmann and Floudas (1987). The existing configuration with the nominal data is presented in Figure 1a and the variation ranges of the uncertainties whose are expected in two hot and C1 stream inlet temperature assumed to be ± 20 K. For enough degree of freedom, the existing configuration involves a bypass with specified fraction.

According to the proposed method, the disturbance sample performance and the results of dynamic optimization problem are obtained firstly. From Figure 1b, it can be seen that these disturbances samples are well distributed, which should be able to represent the uncertain operation condition. The above results focus on the variations of stream output temperatures which can be seen in Figure 1c. Only two stream output temperatures are greatly affected by the disturbances, and H1, C2 stream output temperatures do not appear any apparent variation since the existing structure has sufficient degree of freedom. The generalized critical operating points for $T_{H1,out}$, $T_{H2,out}$ and $T_{C1,out}$ are identified as (614.77, 567.45, 399.21), (603.86, 568.28, 405.68). The network configuration optimization is performed in these two points successively which is shown in Figure 2a and Figure 2b. The coloured unit denotes the purchased one and the unit with dotted line is the existed one. The area variation of existed units is described by the double circle.

Contrast to the existing configuration, the optimized one can handle stochastic and time-dependent operating uncertainties and thus is provided with dynamic flexibility essentially. It is noted that dynamic flexibility index fails to evaluate the degree of dynamic flexibility since it will calculate on every critical operating point which will lead to greater computation burden and the over-synthesis degree cannot be contained. Besides, since the time-varied disturbances following a certain function are not involved in configuration optimization of this case, thus the analysis of the network's response curves with step changes can be added for proving the usefulness of this developed method. The comparison between regular and advanced control strategy is employed to thoroughly analyse the above curves, i.e. Model Predictive Control (MPC) and Proportional Integral Differential Control (PID).

In the following analysis, the bypass K1 is selected as the MV and the controlled variable (CV) is H1 stream output temperature. From Figure 3a, MPC can introduce smooth variation and smaller deviation to the output temperatures under the assumption of step change (t = 1 s, T_{C1,out} = 323K), and although PID bring about greater fluctuation on the beginning of regulation it still gives preferable steady state deviation. It implies that this gradual optimization can make the network effectively away from the instability and circumvent the timedependent realizations in the disturbances. Thus, the future integration problem will not demand significant efforts from the control design system and then the computation burden will be lightened accordingly. Figure 3b denotes that the different influence of the regulation for H1 stream output temperatures of the existing network configuration and the first optimized network configuration on the uncontrolled stream output temperature (C2). Except for the unchanged situation caused by PID, MPC for the regulation of the other stream output temperature can still bring about the variation in better direction. It implies that the previous comparison that MPC can give preferable performance does not merely result from its greater computation burden, i.e. it involves various considerations. Therefore, the proposed integration problem needs to consider MPC featuring advanced control strategy for superior economic and control performance. Besides, the comparison between response curves of the first (subscripted or) and the second (subscripted op) optimal network with the same control strategy is shown in Figure 3c. Regardless of the difference of response time, MPC can give preferable performance on either the first or second optimized configuration since the first optimized configuration has been provided with the capacity of maintaining the disturbances. This difference denotes that the complexity of different structures brings about different uncertainty which exists in the HENs and is expanded by the interaction among the streams. The mutual influence between network configuration and dynamic optimization, thus the dynamic flexible network cannot correspond to the network having perfect control performance. It implies that there will be a trade-off between dynamic flexible and preferable control performance, which is also the key point of the future integration problem. Moreover, the situation that control optimizations for response time and the others parameters are not contained in this paper may be the other reason that the second optimized configuration cannot introduce preferable control performance. Similarly, the greater control action brought by PID is also influenced by the over-synthesis degree. Although it cannot reflect superior control performance, the PID still has desirable calculation time. This also needs to be considered in the subsequent integration problem.



Figure 2a: Optimized heat exchanger network in the first generalized critical operating point.



Figure 2b: Optimized heat exchanger network in the second generalized critical operating point.



Figure 3a: Response curves of the optimal network with different control strategies.



Figure 3b: Influence of different networks on the other stream output temperature.



Figure 3c: Comparison between the two optimal networks with the same control strategy.

4. Conclusions

The conventional flexibility synthesis design has been only implemented by following the stochastic disturbances. The optimality of HENs is largely deviated by the time-dependent realizations in the disturbances. This paper considers the combination of these two types of disturbances to describe the practical operating condition appropriately and the generalized critical operating points are defined to perform the network optimization gradually. The optimized result can denote dynamic flexibility with ensuring certain over-synthesis degree and can be the basis of integration of dynamic flexible synthesis and advanced control designs. Besides, this method which is developed sequentially can lighten calculation burden and reduce difficulty of integration with control design. When severe variability appears on the HENs, significant efforts will not be demanded from the control system in order to maintain stream output temperature around their set points.

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