Estimating the Maximum Possible Correction Factor by Using the High Temperature Differences within Pinch Analysis as Obtained from Practical Experience

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Abstract
Pinch analysis is a very useful method that can increase the energy efficiencies of individual chemical processes including simultaneous heat integration and process optimisation. Pinch analysis is based on constant heat capacity flow (CF) for each stream. In regard to greater temperature differences of more than 200 K, the heat capacity flow could be corrected using a quantified maximal possible correction factor (f_{cor}) obtained from practical experience. This is because of certain determined changes in specific heat capacity (c_{p}), as it is temperature dependent. The correction factor for heat capacity flow is calculated by determining the errors of specific heat capacities. This technique includes those specific heat capacity errors during significant temperature differences that cause errors regarding heat capacity flow. The correction factor could be reduced by using the calculated mistake of heat flow rate during integrated networks. The novelty of this paper is the correction factor, which could be:

- Obtained from practical experience
- Reduced the mistake of heat flow rate
- Reduced the energy loss.

Keywords: Thermodynamic method; Pinch analysis; Heat capacity flow rate; Specific heat capacity

Abbreviation: c_{p}: Specific heat capacity; CF: Heat capacity flow; E: error; f_{cor}: Maximal possible correction factor; k: Slope; n: Constant; q: Mass flow; Φ: Heat flow rate; ∆T: Temperature difference

Introduction
Pinch analysis can increase the energy efficiencies of individual chemical processes. It has established itself as a highly versatile tool for process design. Originally pioneered as a technique for reducing the energy costs of new plants, it was later adapted for retrofits [1]. Pinch analysis quickly proposes good ideas for heat integration during complex processes, e.g. by using a grand-composite curve. A combined heat and power design adds degrees of freedom to the optimisation method.

Pinch techniques are used within the chemical industry for improving heat integration regarding utility systems. Ahmad and Hui [2] extended the concept for direct and indirect integration. Using site-source and site-sink profiles, the targets for steam generation and utilisation between processes were set by Dhole and Linnhoff [3]. Hui and Ahmad [4] developed a procedure for the optimum cost integrations of different processes using exergetic steam costing.

Over the last four decades, the problem of designing and synthesizing optimal HENs (heat exchanger networks) has been the focus of an extensive number of studies [5,6]. In regard to this problem, a set of hot streams at a set of initial (stream) temperatures needs to be cooled in order to correspond to a set of target temperatures, and a set of cold streams at a set of initial (stream) temperatures needs to be heated to another corresponding set of target temperatures. The objective is to determine the structure of the HEN and associated heat exchanger (HEX) heat load/duty (I), together with additional heaters and coolers (utilities), if required. This brings all streams to their target temperatures provided that the HEN’s and HEX’s input and output temperature differentials are greater than or equal to the HEN minimum temperature-differential approach (ΔT_{min}) [6].

A heat exchanger network’s design may depend on the heat-pinch targeting stage, as an approach whereby hot and cold composite curves (CCs) are used for determining the heat energy targets (heat recovery, cold utility, and hot utility) at a specified minimum temperature differential ΔT_{min} [7]. The targeting stage allows the designer of HENs to determine the best performance achievable prior to actual synthesis. Energy targets may be set using CCs, where the minimum hot and cold utilities’ requirements are determined.

Over past decades, pinch analysis techniques have been used for the systematic designing of heat recovery and material conservation systems [8], and within process plants [9]. In particular, pinch analysis is widely used within the area of resource conservation, such as the recoveries of solvents [8], water [10,11], utility gas [12,13], and property-based integration [14,15]. This family of techniques is complementary to mathematical optimisation techniques, as they offer advantages with respect to problem analysis and visualisation. In addition, they also provide useful insights and performance targets for facilitating the subsequent detailed design stage.

Sometimes different correction factors are used that are inserted

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within the models. An equation of state is a thermodynamic equation that relates two or more state functions (temperature, pressure, volume etc.) in order to describe the properties of fluids and their mixtures. The use of cubic equations of state (CEOS) became popular during the modelling of natural gas systems in the 1970s because of their remarkable prediction regarding the phase behaviour of hydrocarbon fluids. Gopal and Biegler [16] presented a phase-equilibrium formulation that handles missing or disappearing phases, and can be extended for incorporating cubic equations of state (CEOS) within a thermodynamic model. It shows that the derivative constraints for the CEOS can be relaxed using the same slack variables that handle the missing phases. Kamath et al. [17] proposed a new general equation-oriented (EO) approach for selecting the appropriate root of the cubic equation of state (CEOS) by incorporating those derivative constraints specific to the desired (vapour or liquid) phase.

A new equation-oriented process model for multi-stream heat exchangers (MHEX) is presented with special emphasis on handling phase changes. This model internally uses the pinch concept in order to ensure minimum driving force criteria. Streams capable of phase change are split into sub-streams corresponding to each of the phases [18].

Heat integration of efficient energy plays an important role within process industries, therefore it is very important to include correction factors within the industrial models. This paper presents a technique for the estimation of a correction factor for specific heat capacity where heat integration is performed over very high temperature differences of more than 200 K.

Methods and Results

Estimating the maximal possible correction factor within pinch analysis as obtained from practical experience

The quantified maximal possible correction factor ($f_{cor}$) estimation for heat capacity flow within pinch analysis could be determined using a specific heat capacity during greater temperature differences of more than 200 K. This correction factor is used for correcting the heat capacity flow used during pinch heat integration. All the basic principles and rules of pinch analysis remain the same.

Pinch analysis treats the streams as a whole and calculates the heat capacity flows ($CF$) of streams. The basic principles of pinch analysis do not consider the phase changes of individual streams particularly and are, therefore not the principle correction factors that take over all the rules of pinch analysis. In the case of a stream's division into multiple streams, these correction factors would only be used if the temperature difference were greater than 200 K. A temperature difference of about 50 K does not cause any errors of $CF$, therefore it does not need any corrections. The correction factor would only be used if the temperature differences were greater than 200 K.

Pinch analysis is a methodology for minimising the energy consumptions of chemical processes by calculating thermodynamically-feasible energy targets, and achieving them by optimising heat recovery systems, energy supply methods, and process operating conditions.

The basic equation of pinch analysis is equation number 1, which presents the heat flow rate ($\Phi$) that depends on the specific heat capacity at a constant pressure for components ($c_p$), mass flow ($q_i$), and temperature difference $\Delta T$ [1,19].

$$\Phi = c_p \cdot q_i \cdot \Delta T = CF \cdot \Delta T$$  \hspace{1cm} (1)

The product of specific heat capacity at a constant pressure of components ($c_p$) and mass flow ($q_i$), denotes the heat capacity flow ($CF$) that is constant for each stream [1]. $CF$ shows a slope for the function of the heat flow rate ($\Phi$) and the temperature difference ($\Delta T$).

These data ($\Phi$, $\Delta T$, and $CF$) are combined for all the streams within the plant for providing composite curves, one for all hot streams (releasing heat) and one for all cold streams (requiring heat). The point of the closest approach between the hot and cold composite curves is the pinch point (or just pinch) with a hot stream pinch temperature and a cold stream pinch temperature. These data ($\Phi$, $\Delta T$, and $CF$) are the bases for determining all the characteristics of pinch analysis, therefore, it is necessary to prevent any errors, especially when determining the heat capacity flow ($CF$):

$$CF = \frac{\Phi}{\Delta T}$$  \hspace{1cm} (2)

The determination of $CF$ can cause errors but only under greater temperature differences of more than 200 K because of certain determined changes in specific heat capacity ($c_p$). The specific heat capacity is defined as the heat required to raise one unit mass of substance by one degree of temperature, therefore it is temperature dependent. The specific heat capacity is the measurable physical quantity that characterises the amount of heat required to change a substance's temperature by a given amount. The correction factor does not include the impact of fluid turbulence.

Estimating a correction factor

For a stream with a high $\Delta T$ of more than 200 K, the calculated heat capacity flow ($CF$) obtained by using equation 2 is inaccurate, therefore the calculated $CF$ could be corrected using the maximal possible correction factor ($f_{cor}$, in W/K), especially, if the total heat flow rate of this stream splits into smaller parts:

$$CF_{cor} = CF \pm f_{cor}$$  \hspace{1cm} (3)

A correction factor provides the calculation of error ($E$) for the heat capacity flow under greater temperature differences of more than 200 K. Figure 1 presents all the basic characteristics of the correction factor, including any necessary new parameters and graphical design. The calculated $CF$ coincides with a value of about half of the temperature difference ($\Delta T/2$) (Figure 1). The maximal errors ($E_{max}$) have to be specially calculated at the left and right sides of the temperature intervals (Figure 1). The $E_{max}$ on the left side from the calculated $CF$ (equation 2) is negative and positive on the right side from the calculated $CF$.

The total temperature interval ($\Delta T$) is divided into lower temperature intervals for a lower value of about $\Delta T = 50^\circ C$ (or smaller) because a temperature difference of about 50 K does not cause any errors of $CF$.

For each temperature interval ($i=1,...,I$) the specific heat capacity ($c_{pi}$) has to be determined and then the differences between these specific heat capacities ($\Delta c_{pi}$), and then their specific heat capacity changes of one degree of temperature ($c_{pi,i}$), are calculated:

$$c_{p,i} - T_{i,1} = \Delta c_{p,i} / \Delta T_{i}$$  \hspace{1cm} (4)

The maximal specific heat capacity change by one degree of temperature ($c_{p,max}$ in J/kgK) is selected, which is then multiplied by the mass flow ($q_i$), and so gives the maximal error ($E_{max}$ in W/K):

$$E_{max} = c_{p} - T_{max} \cdot q_i$$  \hspace{1cm} (5)

The left maximum error ($-E_{max}$ in W/K) and on the right the maximum error ($E_{max}$ in W/K) can be calculated (Figure 1), having the same quantities but different signs. Through three important points
(\(E_{max}\), the calculated \(CF\), \(E_{p,i}\); Figure 1), a line with a known linear function \(E\) (equation 6) can be drawn by using the two points \((E=-E_{max}, \Delta T=0)\), and \((E=+E_{max}, \Delta T=T_{max})\). The \(E\) errors denote the different errors between the limits of the left \((-E_{max})\) and right maximal errors \((+E_{max})\):

\[E_i = k \cdot \Delta T_i + n\]  

(6)

Constant \(k\) determines the slope of the line and constant \(n\) determines the \(y\)-intercept.

The correction factor is determined by using equation 7

\[f_{cor} = E_i \cdot \Delta T_i = (k \cdot \Delta T_i + n) \cdot \Delta T_i\]  

(7)

The correction factor can be calculated by using equation 7 as a function of the temperature difference \((\Delta T_i)\), and by the known parameters of \(k\) and \(n\).

This method can calculate the correction factor, which is then used to correct heat capacity flow during pinch heat integration, without changing the basic principles and rules of pinch analysis.

Case study

The idea for this method was spawned within an existing methanol production plant, where deviation took place between the estimated and real integration mass flow rates.

The low-pressure methanol process, as in this case study, is composed of three subsystems:

- Production of synthesis gas
- Production of crude methanol
- Purification of methanol, which is not presented

All the subsystems were optimised, except the synthesis gas production (only one non-optimal subsystem heating of the natural gas and cooling of the synthesis gas (Figure 2 and Table 1).

The raw material was natural gas, which was heated-up in a steam reformer (REA-1), where synthesis gas was produced from natural gas and steam at 825°C and 15 bar (Figure 2).

3C\(_2\)H\(_4\)+6.5H\(_2\)O \(\rightarrow\) 2CO\(_2\)+12H\(_2\)+1.75CH\(_4\)+2.25CO\(_2\)  
\(\Delta H^{298}=196.17\text{kJ/mol}\) (R1)

3C\(_2\)H\(_4\)+10H\(_2\)O \(\rightarrow\) 3CO\(_2\)+17H\(_2\)+3CO+2.5CH\(_4\)  
\(\Delta H^{298}=277.88\text{kJ/mol}\) (R2)

\(\text{CH}_4 + \text{H}_2\text{O} \rightleftharpoons \text{CO} + \text{H}_2\text{O} \quad \Delta H^{298} = 206.08\text{kJ/mol}\) (R4)

\(\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2\)  
\(\Delta H^{298} = -41.17\text{kJ/mol}\) (R5)

The hot-stream of synthesis gas was cooled within an E107 boiler, in the E109, E110, E111 heat-exchangers with an EA101 air-cooler, and in an E112 water-cooler. The condensate was expanded in flashes: F1, F2, F107, and F108. All the condensates were collected (K1—K5) during the process.

The process shown in Figure 2 was optimised very well, except for only one non-optimal subsystem, for the heating of the natural gas and the cooling of the synthesis gas (Table 1). This subsystem included an existing stream E109-c with a very significant temperature difference.

The need for factorizing the correlation was started after integration of the existing stream E109-c with the EA101 stream because there was insufficient heat flow rate.

The existing stream E109-c had a large temperature difference (\(\Delta T=400\) K). The calculated \(CF\) caused inaccurate values for real problems if the heat flow rate of E109-c was integrated within several parts. The calculated \(CF\) for the existing stream E109-c was corrected by a correction factor.

**Integration using calculated \(CF\)**

The hot and cold streams of the existing synthesis gas process are presented in Table 1. Integration was carried out after all the parameters.
(Φ, ΔT and CF) were known. The calculated heat capacity flow rate of the stream E109-c (CF) by using equation 2 was 8309 W/K. This stream was integrated within the hot streams EA101 for 897.4 kJ and partly with E109-h for 2426.3 kJ, by using ΔT_{mi} = 20°C (Figure 3).

**Integration by using corrected CF**

The total temperature interval (ΔT=400 K) of stream E109-c was divided into lower temperature intervals for a rounder lower value (ΔT=50°C, Figure 4). For each temperature interval (i=1,…8) the specific heat had to be a determined capacity (c_{p,i}) and then the difference between these specific heat capacities (∆c_{p,i}) and those of the specific heat had to be a determined capacity (c_{p,i}) and then the value (∆c_{p,i}) was calculated by using equation 4. The maximal specific heat capacity changed by one degree of temperature (c_{p-T,max}=108 K) because this was the first possible temperature difference (Figure 4). The mass flow (q_{E109-c}) of E109-c was 2.9241 kg/s. The maximal error (E_{mi}) was 10.30 W/K by using equation 5. E109-c was divided at ΔT_{i} to 108 K because this was the first possible temperature difference for integration with EA101 (Figure 3).

The linear function of errors (E_{i} in W/K; equation 6) was obtained by using two points (E_{109-c} = 10.3, ΔT_{i}=20°C) and (E_{109-c} = 0.0515, ΔT_{i}=108 K): E_{i} = k \cdot ΔT_{i} + n=0.0515 \cdot ΔT_{i}−10.3 \quad (8)

The correction factor for E109-c was determined by using equation 7:

\( f_{cor} = E_{i} \cdot \Delta T_{i} = (0.0515 \cdot 108.3 - 10.3) = -511.7 \text{ W/K} \quad (9) \)

The calculated heat capacity flow rate of the stream E109-c (CF) was 8309 W/K and the new remaining correct CF_{cor} was 7797.3 W/K:

\( CF_{cor} = CF \pm f_{cor} = 8309 - 511.7 = 7797.3 \text{ W/K} \quad (10) \)

The difference between the calculated CF and the corrected CF_{cor} was 6%. New integration was performed by using the corrected (CF_{cor}). The cold E109-c stream was integrated with EA101 for 842 kW and partly with E109-h for 2481.7 kW at ΔT_{mi} = 20°C, by using the correction factor (Figure 5). The integration heat flow rate (Φ) between E109-c and EA101 was 897.4 kW when using conventional pinch analysis. The integration heat flow rate (Φ) between E109-c and EA101 was 842 kW when using the correction factor. The heat flow rate calculated after the correction factor was comparable with the real retrofit.

This was confirmed by using practical experience that the correction factor was only required when ΔT was greater by more than 200 K because the errors (E) were becoming greater. Thereby, the optimal lengths for the temperature intervals (ΔT_{opt}) could be determined that did not require correction. The optimal length of the temperature intervals (ΔT_{opt}) could be determined by using a graphical method (Figure 6). The left and right maximum errors (E_{mi}) were halved to the linear line (E) and thereby denoted the points A and B. All temperature intervals between points A and B were summed and determined an optimal length for the temperature intervals (ΔT_{opt} of about 200 K. Thus also providing that errors (E) were no greater than 5 W/K.

**Conclusion**

The correction factor obtained from practical experience can reduce heat integration errors within a pinch analysis method. Pinch analysis does not guarantee a global optimum solution but it quickly proposes good ideas for heat integration during the process, therefore the accuracy and reliability of this method is even more important. The correction factor allows for quick adjustments of the heat capacity flow. This correction factor includes maximal specific heat capacity error during a significant temperature difference of more than 200 K, which causes errors regarding heat capacity flow. This correction factor reduces these errors and thus allows for better integration, which is highly comparable with the real data. This correction factor could be
extended in the future with other effects (such as pressure).

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