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An algorithm for optimal waste heat recovery from chemical processes

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ABSTRACT

We describe a computer algorithm designed to calculate the optimal energy extraction in the form of heat used for steam raising from chemical processes. The concepts are illustrated using chemical plant stream data in a process with multiple distillation columns. Pinch analysis is first applied to find the grand composite curve (GCC) of the problem, which is then used by the algorithm to determine the maximum mass flow rate of steam that can be produced from process waste heat. An analysis of the effects of the minimum temperature of approach ΔT_{min} on the optimal steam raising result is also conducted, and it is found that, in general, a higher ΔT_{min} will reduce the percentage heat recovery from the process.

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1. Introduction

Large-scale chemical processes require significant energy inputs to operate effectively. Reduction of these inputs, or recovery of waste heat, can therefore yield significant economic and environmental advantages. One way of improving the energy efficiency of a process is *pinch analysis* (Kemp, 2007), which involves the transfer of internal heat between process streams to reduce external heat requirements. Introduced by Hohmann (1971) and furthered in the work of Umeda et al. (1979), Linnhoff et al. (1983) and others (Linnhoff et al., 1982; Linnhoff and Hindmarsh, 1983; Kemp and Deakin, 1989; Ahmad and Linnhoff, 1989; Shenoy, 1995; Kemp, 1991; Smith, 2005), this approach allows the determination of the minimum external energy required to run a process. Inputs required for this approach include initial temperatures, final temperatures, flow rates and specific heat (*CP*) values of process streams. The pinch method has been used to successfully identify process inefficiencies and retrofit plants into more cost-effective and energy-efficient designs, including in industrial milk-powder production (Walmsley et al., 2013) and ethanol distillation (Gu et al., 2006). It forms part of the modern process design toolbox, as a complement, for example, to design approaches, like residue map analysis, for optimizing separation trains in flowsheets (Biegler et al., 1997).

Pinch analysis does not remove the need for external heating and cooling and, in general, waste heat at lower temperatures has to be rejected by the process. This introduces the possibility of waste heat recovery which has significant energy efficiency implications. If the waste heat is low-grade, it is difficult to recover and requires the use of complex heat transfer methods such as the organic Rankine cycle (Law et al., 2013; Little and Garimella, 2011). However, if high-grade heat is available within the process, it can potentially be extracted in the form of steam. In this paper, the maximum amount of steam that can be recovered from a pinch analysis-optimized process is calculated using a novel algorithm which shows that the optimal pathway for energy recovery involves countercurrent heat removal below the process pinch. Concerns related to the detailed design of heat exchangers and boilers used to produce steam are not addressed – the final heat exchanger network is not analyzed given that significant research has gone into such topics (Aegerter, 2005). Instead, our goal is to provide a method for calculating the optimum heat recovery which can then be used as a starting point for the detailed design of the particular heat exchanger network.

The optimization result from pinch analysis requires that only coolers are added below the pinch temperature. Since steam raising requires removing heat from the process, it becomes in the language of pinch technology analogous to placing a cooler below the

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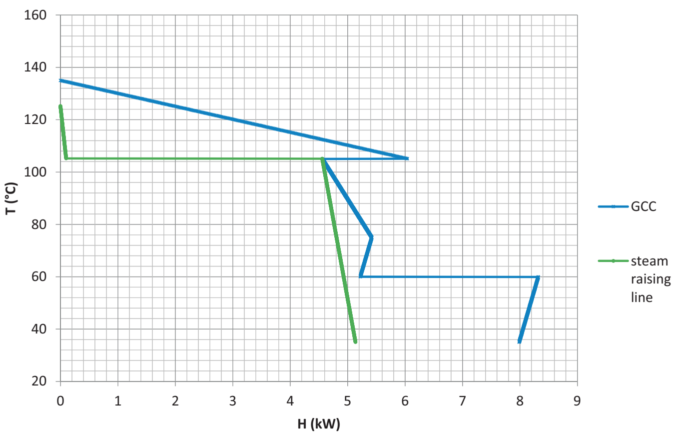

Fig. 1. Example of GCC and steam raising line. 1: (H_{start}, T_{start}); 2: (T_{gccmin}); 3: (H_{wsat}, T_{sat}); 4: (H_{ssat}, T_{sat}); 5: (0, T_{final}).

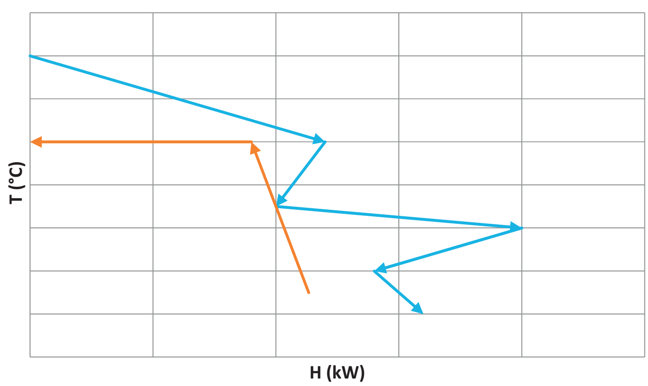

Fig. 2. Countercurrent pathway.

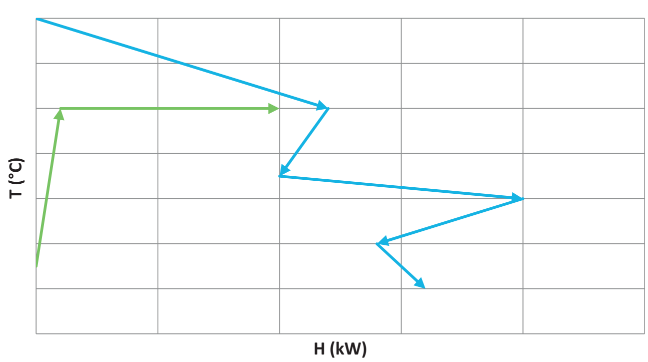

Fig. 3. Concurrent pathway.

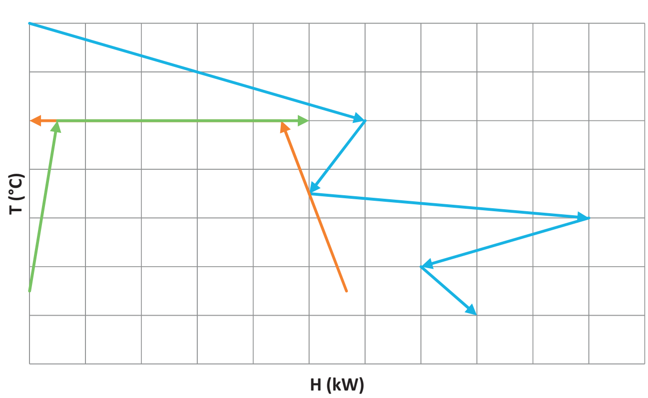

Fig. 4. Case I.

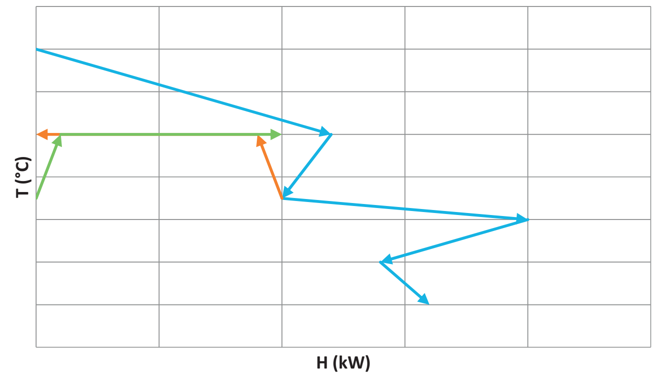

Fig. 5. Case II.

pinch. This is always possible to do without affecting the original pinch point. Herein, a novel algorithm is reported to calculate the maximum possible mass flow rate of steam at a given temperature and pressure that can be recovered from the process under these conditions.

Using this approach process engineers will be able to optimize the conditions for recovering waste energy from processes which also has a salutary environmental effect in that it reduces emissions generated by conventional power generation plants for the process use. The algorithm is designed to analyze complex processes including multiple streams, and steam generation at varied pressures and temperatures conditions

2. Methodology and corresponding algorithm

2.1. Summary of approach

A water mass balance shows that for the extraction of the maximum amount of heat in the form of steam the mass flow rate of water at all three heating stages (sensible, latent and superheating) must be the same. The algorithm we propose calculates a solution that fulfills this condition and the solution is checked to ensure that it does not create a new pinch.

2.2. Mathematical derivation

At each temperature level on the grand composite curve below the pinch, there is a maximum amount of energy that can be extracted while maintaining the optimal minimum energy requirement (MER) result. In order to use the maximum amount of energy without changing the pinch, it must be determined whether or not the steam raising lines intersect with any segment of the Grand Composite Curve (GCC) below the pinch. Any crossing of the GCC would violate the pinch temperature condition which is not allowed. All the variables used in the following analysis are shown in the schematic in Fig. 1.

In order to determine if the GCC and steam raising lines cross, the equations representing them need to be derived first. The straight line segments on the GCC can be represented using the following equation:

$$\frac{T - T_1}{H - H_1} = \frac{T_2 - T_1}{H_2 - H_1} \tag{1}$$

where (H_1, T_1) and (H_2, T_2) stand for the starting and ending point of any GCC line segments. The slope of the line segments along the GCC (in temperature-enthalpy, T–H coordinates) is given by

$$\frac{1}{C_{pw} \times M_w} = \text{Absolute value} \quad (\text{slope}) \tag{2}$$

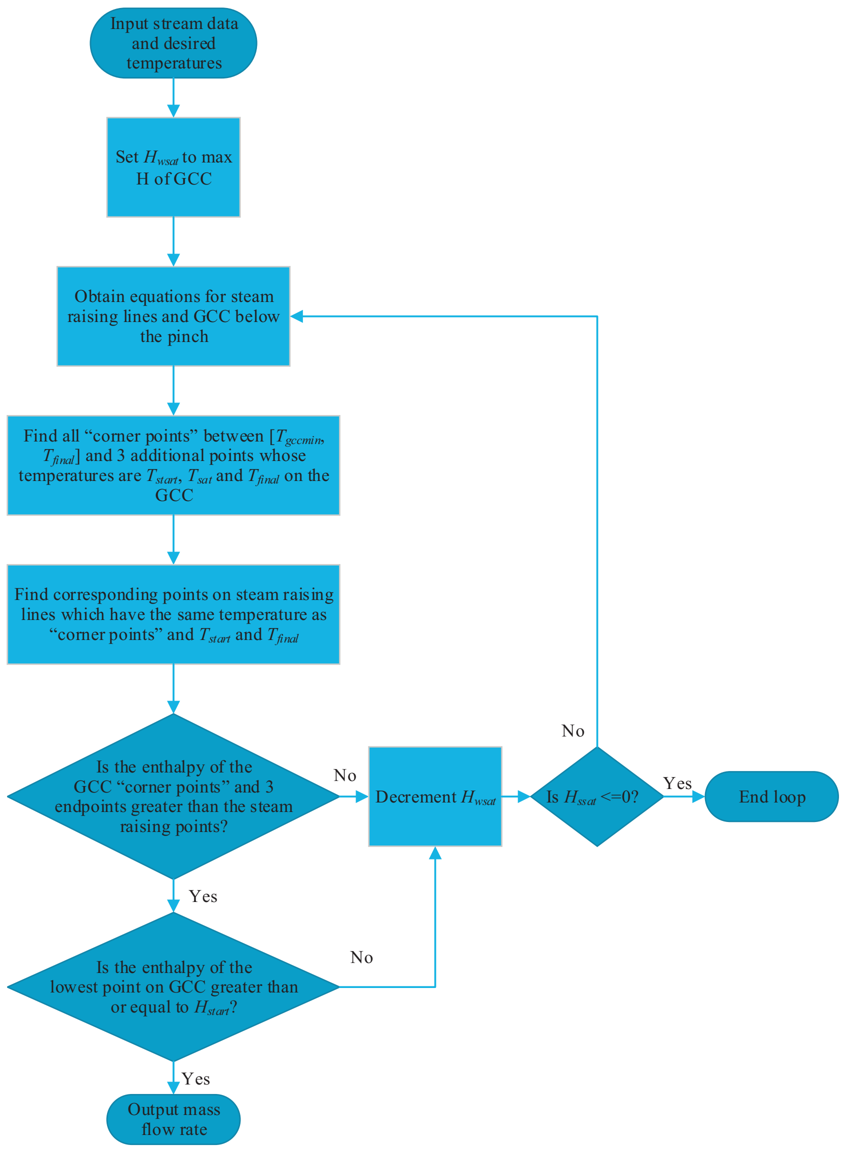

Fig. 6. Algorithm flow chart.

Here C_{pw} is the heat capacity of water in kJ/kg °C and M_w is the mass flow rate of steam in Kg/s. For the sensible heat stage, M_w is given by

$$M_w = \frac{1}{C_{pw}} \times \frac{H_{start} - H_{wsat}}{T_{sat} - T_{start}} \quad (3)$$

where H_{start} is the enthalpy of the inlet water in KW, H_{wsat} is the enthalpy of saturated water in KW, T_{sat} is the water vaporization temperature in °C and T_{start} is the water inlet temperature in °C.

For the latent heat stage, M_w is given by

$$M_w = \frac{H_{wsat} - H_{ssat}}{\Delta H_{vap}} \quad (4)$$

H_{ssat} is the enthalpy of saturated steam in KW and ΔH_{vap} is the vaporization enthalpy of water in kJ/kg.

For the superheating stage, ΔH_{vap} is given by

$$M_w = \frac{1}{C_{ps}} \times \frac{H_{ssat}}{T_{final} - T_{sat}} \quad (5)$$

C_{ps} is the heat capacity of steam in kJ/kg °C and T_{final} is the final temperature of steam in °C. The three equations for M_w contain four unknowns (the temperatures of all stages are input before the computation begins), which are H_{start}, H_{wsat}, H_{ssat} and M_w. In order to solve this problem, one of the unknowns must be assumed; we chose H_{wsat}. Eqs. (6)–(8) are found by rearranging Eqs. (3)–(5) in terms of H_{wsat}.

$$H_{ssat} = C_{ps} \times H_{wsat} \times \frac{T_{final} - T_{sat}}{\Delta H_{vap} + C_{ps} \times (T_{final} - T_{sat})} \quad (6)$$

$$H_{start} = H_{wsat} \times \left(1 + C_{pw} \times \frac{T_{sat} - T_{start}}{\Delta H_{vap}}\right) - H_{wsat} \times \left(C_{pw} \times C_{ps} \times \frac{T_{sat} - T_{start}}{\Delta H_{vap}}\right) \times \left(\frac{T_{final} - T_{sat}}{\Delta H_{vap} + C_{ps} \times (T_{final} - T_{sat})}\right) \quad (7)$$

$$M_w = \frac{H_{wsat}}{\Delta H_{vap}} \times \left(1 - C_{ps} \times \frac{T_{final} - T_{sat}}{\Delta H_{vap} + C_{ps} \times (T_{final} - T_{sat})}\right) \quad (8)$$

Here H_{wsat} is first assumed to be the maximum enthalpy that appears among all data points below the pinch as a conservative

Table 1
Stream data for the toluene plant.

Flow rate (kmol/h)	H2	TOL	MTO	M10	F11	F10	R10	E21	E20	DIV	DIL
Toluene	0	10.9	16.16	17.07	17.07	17.07	9.35	9.35	9.35	0.92	8.43
Benzene	0	0	3.42	4.24	4.24	4.24	8.10	8.10	8.10	0.82	7.28
Xylene	0	0	3.32	3.45	3.45	3.45	7.31	7.31	7.31	0.12	7.18
Hydrogen	2.00	0	0	82.00	82.00	82.00	82.00	82.00	82.00	80.00	2.00
Total flow	2.00	10.90	22.90	106.76	106.76	106.76	106.76	106.76	106.76	81.86	24.90
Temp (C)	25.0	25.0	25.0	35.5	129.0	450.0	450.0	300.0	40.0	40.0	40.0
Pres (bar)	1.0	1.0	1.0	10.0	10.0	35.0	35.0	35.0	10.0	10.0	10.0
Enthalpy (kW)	0.0	36.4	78.0	116.5	431.1	1127.7	1128.5	813.9	127.4	33.6	94.2
Flow rate (kmol/h)	**E30**	**T1V**	**E40**	**Offgas**	**D2L**	**T1L**	**T2F**	**T2V**	**E60**	**SO**	**BENZENE**
Toluene	8.43	0	0	0	0	8.43	8.43	0	0	0	0
Benzene	7.28	0.50	0.50	0.22	0.28	7.06	7.06	2.34	2.34	1.58	1.58
Xylene	7.18	0	0	0	0	7.18	7.18	0	0	0	0
Hydrogen	2.00	2.00	2.00	2.00	0	0	0	0	0	0	0
Total flow	24.90	2.50	2.50	2.22	0.28	22.68	22.68	2.34	2.34	1.58	1.58
Temp (C)	75.0	35.5	25.0	20.0	20.0	129.9	80.0	104.5	70.0	70.0	35.0
Pres (bar)	1.5	1.0	1.0	1.0	1.0	2.0	0.5	2.0	2.0	2.0	1.0
Enthalpy (kW)	137.3	11.8	9.5	5	3.7	188.6	131.2	58.6	36	24.2	22.1
Flow rate (kmol/h)	**RT2**	**T2L**	**T3L**	**E120**	**T3V**	**E90**	**RT3**	**Mixed**	**Purge**	**Rec-out**	**Recin**
Toluene	0	8.43	0	0	10.81	10.81	2.38	8.43	3.17	5.26	5.26
Benzene	0.77	5.48	0	0	7.03	7.03	1.55	5.48	2.06	3.42	3.42
Xylene	0	7.18	1.86	1.86	6.83	6.83	1.5	5.33	2.01	3.32	3.32
Hydrogen	0	0	0	0	0	0	0	0	0	0	0
Total flow	0.77	21.10	1.86	1.86	24.68	24.68	5.43	19.24	7.24	12.00	12.00
Temp (C)	70.0	150.3	249.3	25.0	183.2	80.0	80.0	80.0	80.0	80.0	25.0
Pres (bar)	2.0	3.0	1.0	1.0	5.0	2.0	2.0	2.0	2.0	2.0	1.0
Enthalpy (kW)	11.8	184.2	13.6	−12.8	482.3	146.0	32.2	113.9	42.9	71.0	41.6

starting point for the computation. After the value of H_{wsat} is chosen, the other three variables can easily be calculated based on Eqs. (6)–(8) and the steam raising line can be constructed based upon these calculations. Then further calculations are done to determine whether or not the steam raising lines intersect with GCC below the pinch.

2.3. *Determination of the optimal pathway*

Before describing the algorithm for calculating maximum heat recovery, the optimal thermodynamic pathway for steam raising needs to be determined. To obtain steam at a certain temperature using input water at a given temperature, there are at two pathways that could be used: either a countercurrent or concurrent pathway. For the countercurrent pathway, water enters at the right end of the *T*–*H* diagram and its temperature gradually increases as it moves to the left as shown in Fig. 2. For a concurrent pathway, the water enters at the left end of the *T*–*H* diagram and its temperature increases as it moves to the right as shown in Fig. 3.

Figs. 2–5 are used as conceptual demonstrations of these thermodynamic pathways. The two pathways described are similar to those which occur in the condenser of a distillation column in either countercurrent or concurrent operation, where entering cold water becomes hot when condensing the hot vapor emerging from the column.

One of the results we show here using a simple geometric argument is that the concurrent pathway is *never better* than the countercurrent pathway in terms of maximizing heat recovery from the process. This is obvious when the GCC below the pinch involves line segments with negative slopes. However, this is not the usual case and in this situation we use Figs. 4 and 5 to support our arguments. In those figures the orange line represents the countercurrent pathway while the green line represents the concurrent pathway. In both cases there are line segments with positive slopes where the process heat cascade shows a deficit (forming the triangular shapes in these figures). In *Case I* (Fig. 4), the countercurrent pathway is forced to stop where the vertical line from the point A intersects it, since to go beyond that point would take energy from the area similar to that within the triangle C (Fig. 5). This is not allowed since that part of the process is self-sufficient with energy from the hot streams supplying that required by the cold streams. This implies an energy advantage of the countercurrent process illustrated by the line AB. This is always the case with these triangular projections from the GCC. In the *unique situation* where the starting temperature is exactly at a corner point temperature in the GCC, illustrated by *Case II* (Fig. 5), the two pathways are totally symmetric and utilize the same amount of energy, and the corresponding mass flow rates are identical. Thus we conclude that the concurrent pathway cannot utilize heat from the rightward sloping portions of the GCC and therefore cannot provide more steam than the countercurrent pathway. As discussed this unusable heat (shown in Fig. 5 as the region C) cannot be removed from the process and represents a hard boundary. In light of this conclusion the countercurrent pathway is utilized in the following discussion.

Table 2
MER results for the toluene plant at ΔT_{min} = 10 °C.

Q_{Hmin}	2845.5 kW
Q_{Cmin}	2830.5 kW
T_{pinch}	254.3 °C

Table 3
Steam raising results for the toluene plant at ΔT_{min} = 10 °C.

H_{start}	2782.389 kW
H_{wsat}	2469.355 kW
H_{ssat}	53.86507 kW
M_w	1.069838 kg/s
Q_{steam}/Q_{Hmin}	0.764692

2.4. *Algorithm and flow chart*

Before the computation starts, the desired inlet water temperature (T_{start}), water vaporization temperature (T_{sat}), and final temperature of the steam (T_{final}) must be input. Since the water

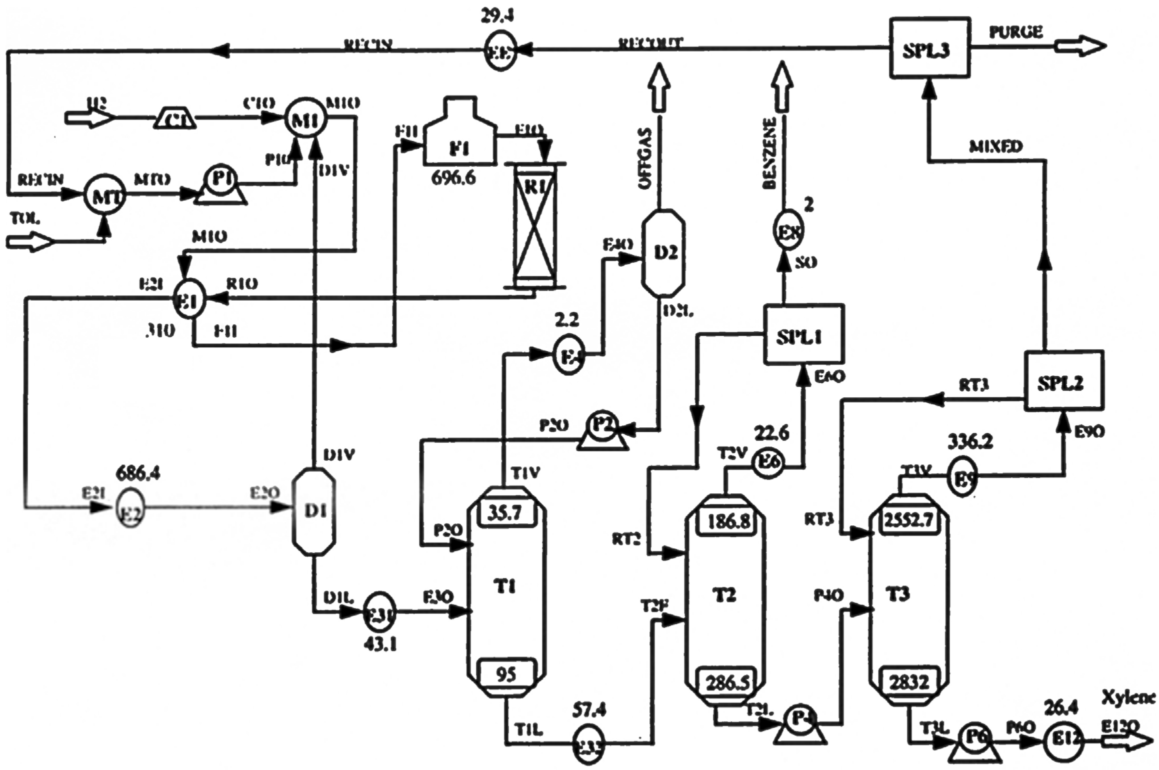

Fig. 7. Process flow diagram for the toluene plant.

stream is also treated as a "cold stream" in our algorithm, input temperatures are automatically adjusted to find the pinch-shifted temperatures (actual temperature + $\Delta T_{min}/2$). In the following discussion, T_{start}, T_{sat} and T_{final} will represent the shifted temperatures for convenience.

To initiate the computation, H_{wsat} is assumed to be the largest enthalpy that appears below the pinch at the beginning. This assumed value is used to find the sensible heat, latent heat and superheating lines which are constructed based on Eqs. (3)–(5). It must then be verified that this solution does not cross the GCC. To do this, "corner points" between the desired temperature range, *i.e.* [T_{gccmin}, T_{final}] and three additional points on the GCC whose temperatures are T_{start}, T_{sat} and T_{final} are identified. Corresponding points on the steam raising line with those temperatures must be found using Eqs. (3)–(5). The GCC "corner points" and three endpoints are then compared with the corresponding steam raising points. If all "corner points" and three endpoints are greater or equal to the corresponding points on the steam raising line, *then*

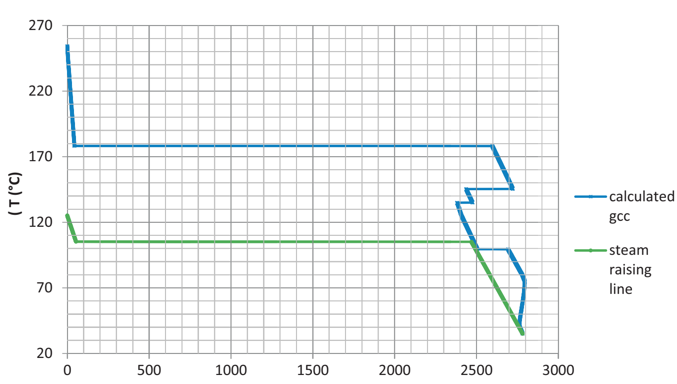

Fig. 8. GCC and optimal steam raising line for the toluene plant.

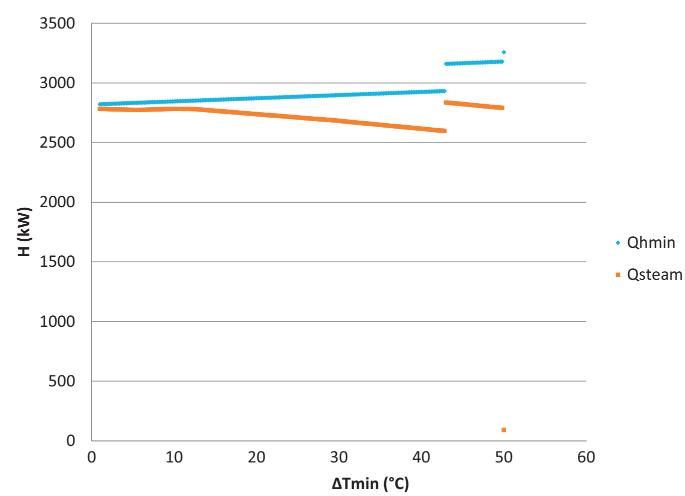

Fig. 9. Q_{Hmin} and Q_{steam} as a function of ΔT_{min} for the toluene plant.

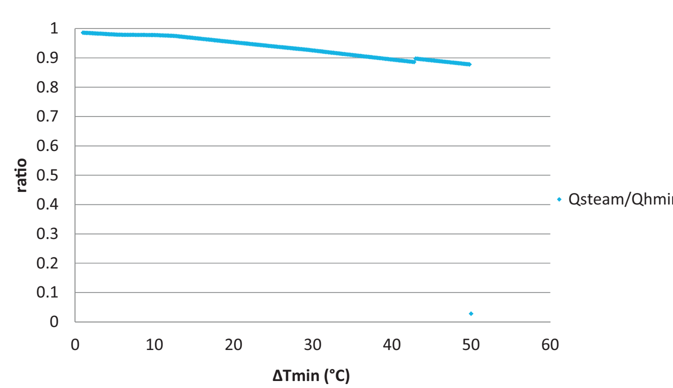

Fig. 10. Heat recovery ratio for varying ΔT_{min} for the toluene plant.

the pinch is not violated. If they do intersect, H_{wsat} is decreased by a small amount, *e.g.* 0.01 kW, and the above process is repeated until the 'no-crossing' criterion is met and the optimum steam raising line is thus found. When H_{ssat} reaches zero, the loop will stop automatically, implying, in this situation, that no solution is possible with the given inputs.

Finally, the lowest point on the steam raising line, H_{start} must be checked against the lowest temperature point on the GCC. This is because H_{start} represents the total energy removed from the GCC, effectively shifting all of the GCC lower than T_{start} leftward by H_{start}. If H_{start} is greater than the lowest point on the GCC, a new pinch would be created and the solution is invalid. It is also important to note that only heat below the pinch can be used, so T_{final} must be lower than T_{pinch}. Fig. 6 shows a flow chart representation of this algorithm.

3. Results and discussion

The algorithm above was coded using Microsoft Visual Basic. Stream temperatures, CP values, and ΔT_{min} are inputs for the program whose output is the maximum steam that can be produced from the process waste heat.

We used a toluene disproportion plant taken from Hengstebeck and Banchero (1969) with its process schematic and stream data shown, respectively, in Fig. 7 and Table 1 in Appendix. After extracting information from the original flowsheet and performing a complete flowsheet simulation to get all the required thermodynamic data required by the pinch design method, we ran the waste heat recovery program using the following data: 12 hot/cold process streams, three distillation columns and ΔT_{min}, T_{start}, T_{sat}, T_{final} fixed at 10 °C, 30 °C, 100 °C and 120 °C, respectively. The pinch calculations yielded MER results shown in Table 2. Fig. 8 shows the corresponding steam raising trajectory given by running our algorithm and Table 3 displays the numerical results obtained. ΔT_{min} was then varied in order to investigate its effect on steam raising and waste heat recovery for this process. An initial value of ΔT_{min} of 1 °C was used and calculations done for increasing temperature increments of 0.2 °C until a value of 50 °C. For each ΔT_{min}, the program determined M_w, Q_{steam} (the amount of energy recovered in the steam raising process), Q_{Hmin} and Q_{Cmin}. Figs. 9 and 10 display the results. The ratio Q_{steam}/Q_{Hmin} was found to decrease as ΔT_{min} increased.

4. Conclusion

We describe an algorithm that leads to the calculation of the maximum amount of steam that can be theoretically raised from waste heat recovery in chemical processes, given flowsheet stream data, the desired steam temperature and pressure, and a value for the minimum temperature approach ΔT_{min} used in the process pinch analysis. This result is useful for improving the energy efficiency of chemical processes by converting waste heat into a useful form. However, it is important to note that the optimal result given here is only an ideal point. Just as the optimal MER result in pinch analysis can be adjusted to account for operational and economic constraints, our approach should be used as a guideline when designing a steam heat recovery system. By working downwards from the optimal result, however, the plant designer can consider the tradeoffs inherent in each revision, and reach a cost-effective solution.

Appendix.

See Table 4.

Table 4
Nomenclature.

T_{start}	Water inlet temperature (°C)
T_{sat}	Water vaporization temperature (°C)
T_{final}	Final temperature of steam (°C)
H_{start}	Enthalpy value of inlet water (kW)
H_{wsat}	Enthalpy value of saturated water (kW)
H_{ssat}	Enthalpy value of saturated steam (kW)
T_{gccmin}	Minimum temperature of the GCC (°C)
CP	Heat capacity multiplied by mass flow rate (kW/°C)
C_{pw}	Heat capacity of water (kJ/kg °C)
C_{ps}	Heat capacity of steam (kJ/kg °C)
ΔT_{min}	Minimum temperature difference between hot and cold streams for heat exchange (°C)
Q_{steam}	Heat transferred to steam from the GCC (kW)
Q_{Hmin}	Minimum external heat required, from MER analysis (kW)
Q_{Cmin}	Minimum external cooling required, from MER analysis (kW)
M_w	Mass flow rate of steam (kg/s)
ΔH_{vap}	Enthalpy of vaporization of water (kJ/kg)
T_{pinch}	Pinch temperature, from MER analysis (°C)

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