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Research article

Modeling and simulation of heat balance and internal heat recovery targets through a combination of stream specific minimum temperature difference and polynomial temperature coefficients of specific heat capacities using pinch analysis

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Abstract: Existing heat balancing and energy targeting model in Pinch Analysis rely on use of interpolated values of specific heat capacities and global values of minimum temperature difference ΔT_{min} , respectively. Even though this model is useful in estimation of the maximum internally recoverable heat recoverable in processing plants, it does not adequately represent the actual state properties of industrial processes. Specific heat capacities of fluids are polynomial functions of temperature of material under processing. The values of ΔT_{min} also vary depending on the nature of the process stream under analysis.

In this study, improvement to the heat balancing and energy targeting processes of pinch analysis was proposed. The study combined the use of stream specific values of ΔT_{min} and polynomial temperature functions of specific heat capacities for heat targeting model. This was coded and executed using a PHP program. The model performance was tested using data from three thermochemical plants, Plant A, B and C, which process linear alkyl benzene sulphonic acid, dairy products and ethanol, respectively.

The proposed method for heat balancing computed more heating requirements for plant A, B and C by 0.37%, 0.65% and 0.72% respectively, compared to the traditional method of heat balancing. The cooling loads for Plant A and B were less by 2.23% and 32.52% respectively, while for Plant C, they were more by 0.64%. The computed internally recoverable heat targets were more

by 1.5%, 4.5% and 2.2% for Plants A, B and C. Simulations of the proposed model were carried out over a range of temperature targets, for different process streams. For gaseous process streams, heating and cooling load requirements were less. Reverse behavior was observed in liquid and steam containing streams, where the heating and cooling load requirements were more.

Keywords: heat balance; pinch analysis; energy targeting; specific heat capacities; polynomial functions; internally recoverable heat; minimum temperature difference; thermochemical plants

1. Introduction

Energy efficiency is one of the interventions currently used in processing plants to reduce production cost. This uses tools like pinch analysis, a process integration technique employed to reduce external heating and cooling duties. Through this tool, process engineers compute thermodynamically feasible heat targets that can be recovered internally and then design a heat exchange network to realize these targets. Pinch analysis is a three-stage process involving heat balancing, energy targeting and design of heat exchange network [1]. Use of pinch analysis enables process engineers to identify the internal heat recovery targets at the process design stage, or during retrofit of a plant.

Since the inception of pinch analysis in the 1970s by Linhoff and Hindmarsh [2], there have been suggested improvements on the tool, which include total site targeting, concepts of the use of stream specific minimum temperature difference (ΔT_{min}) during energy targeting, and combination of mathematical programming and pinch analysis in heat recovery approaches [3]. Conventional methods of pinch analysis however still use global values ΔT_{min} for energy targeting. However, this approach has been said to lead to underestimation or overestimation of internally recoverable heat.

Improvements on heat balancing have been suggested by reference [1] although there is no literature showing that such improvements have been tested. The suggestions focus on the use of polynomial temperature coefficients of specific heat capacities. Current methods of determining the total required heating and cooling in facilities relies on interpolation of specific heat capacities, between the initial and final temperature of the streams. Theoretical experiments on internal combustion engines have demonstrated that the engine power modelled using polynomial temperature coefficients of specific heat capacities are different from that modelled using the interpolated values. Reference [4]'s modeling of an Otto-Cycle engine revealed variations in performance between models that used temperature dependent specific heat capacities and those that used constant specific heat capacities. A similar study by reference [5], but on a naturally aspirated Miller cycle, also showed that accurate predictions of cycle performance can be enhanced by use of a fourth order temperature polynomial of specific heat capacities.

The use of stream specific values of ΔT_{min} was first postulated by reference [2]. Available literature on the use of this method in practical design problems is however not documented. Theoretical tests on the shifting of temperature during energy targeting have shown that indeed the use of stream specific ΔT_{min} yields different results. Example of such studies can be found in reference [6]. In this study, the concept of using stream specific ΔT_{min} was tested on secondary data from a diary plant. The results revealed that the cooling and heating utility targets determined using the stream specific ΔT_{min} were lesser compared to those achieved using the traditional methods.

So far, the suggested improvements for both heat balancing and energy targeting have not gone far enough to determine magnitude of deviations that arise from use of the conventional methods instead of these suggested improvements. The suggested improvements have also not been jointly used. This work attempted to combine the use polynomial temperature coefficients of specific heat capacity and stream specific values of ΔT_{min} in pinch analysis for heat balancing and energy targeting. The results were compared to those modeled using conventional methods.

1.1. Pinch analysis

Heating balancing is the first stage in pinch analysis and is guided by the First Law of Thermodynamics [7]. It entails determination of the total cooling and heating loads for each stream in a processing plant. These loads are then summed up. More details on this process are provided in [2].

The energy targeting stage of pinch analysis is illustrated in reference [1]. In this stage, there are six processes:

- a. Shifting of all stream temperatures by a value of ΔT_{min} .
- b. Creating of the shifted temperature intervals.
- c. Determining streams whose temperature profiles intersect into each shifted temperature interval.
- d. Determining the heat deficit or surplus in each interval, by summing up the enthalpies of each stream that intersects in the interval.
- e. Cascading the heat deficits and surpluses, to a pinch point.
- f. Determining the minimum required external cooling and heating loads in the process plant.

The values used for ΔT_{min} determine the permissible heat exchanged between streams and the size of the heat exchanger. A larger value limits the amount exchanged, thus resulting in higher operating costs. The process plant has to use more utilities to meet cooling and heating demands. As well, smaller values of ΔT_{min} reduce the driving forces for exchange of heat, calling for more exchange area. This increases the cost of heat exchangers [2]. Figure 1 shows an example of such a relationship.



Figure 1. Illustration of effect of ΔT_{min} on costs.

Figure 1 shows that increase in ΔT_{min} increases energy costs of running the facility while a reduction of the same increases the cost of heat exchangers. Optimization of this value is therefore necessary. Where global values of ΔT_{min} are used, an overestimation or underestimation of targets is likely to occur. In practical sense, temperature driving force for heat exchange is different for

different streams, and is mostly dependent on the overall heat transfer coefficient in the process stream [10]. For optimal design variables, it is essential to adopt the ΔT_{min} value specific to each stream in the process plant.

2. Methods

For energy balancing and heat targeting, this study modified the heat exchange formula to include the polynomial temperature coefficients of specific heat capacity, and the heat targeting algorithm to include the use of stream specific ΔT_{min} .

The rate of change of enthalpy in a stream, ΔH is calculated as:

$$\Delta \mathbf{H} = \dot{\mathbf{m}} \times C_p \times \Delta \boldsymbol{\theta} \tag{1}$$

 \dot{m} is the mass flow rate of the process fluid or gas, in kg/s. C_p is the isobaric specific heat capacity, in j/g.K. $\Delta\theta$ is the difference between the source temperature T_s and the target temperature T_t of the stream. Streams with higher T_s than T_t are denoted as hot streams while those with higher T_t than T_s are cold streams. Hot streams require cooling duty. Cold streams require heating duty. The independent variables in Eq (1) are obtained through measurements of each stream in the plant. They can also be obtained from a design data sheet.

In the current model of heat balancing, the value of C_p is determined through interpolation of values that correspond to T_s and T_t . The values thus have some uncertainty [11], which can be addressed by use of polynomial temperature coefficients. Improvements on the use of C_p were suggested by reference [12], suggesting the use of fourth order polynomials of temperature when calculating specific heat capacities. The C_p in this case is presented as:

$$C_p = \mathbf{A} + \mathbf{B}\mathbf{T} + \mathbf{C}T^2 + \mathbf{D}T^3 \tag{2}$$

Here, A, B, C and D are polynomial coefficients and T is instantaneous temperature. These coefficients are different for compounds and have been published by various literature sources, for example, in references [8] and [9].

To calculate ΔH therefore, over a range of temperatures, from the source T_s to final T_t, Eq (1) was expressed as:

$$\Delta H = \dot{m} \int_{T_t}^{T_s} (A + BT + CT^2 + DT^3)$$
(3)

The solution to Eq (3) was expressed as:

$$\Delta H = \dot{m} \left[A(T_s - T_t) + \frac{B}{2} (T_s^2 - T_t^2) + \frac{C}{3} (T_s^3 - T_t^3) + \frac{D}{4} (T_s^4 - T_t^4) \right]$$
(4)

Equation (4) captures the changes in specific heat capacities per change in temperature, thus avoiding the averaging, which might result in deviations from the reality.

Equation (4) was incorporated in the heat balance and energy targeting model, in combination with a step that allowed using the stream specific values of ΔT_{min} . An algorithm was developed for model coding and execution. Figure 2 shows the algorithm.



Figure 2. Heat balance and energy targeting algorithm.

The algorithm uses Celsius scale, because of the polynomial functions presented in equation (4). The second, third and seventh steps incorporated the proposed changes to heat balancing and energy targeting models. The shifting of temperature was unique to each stream, using a stream specific value of ΔT_{min} . Heat balancing incorporated coefficients of A, B and C. Coefficient D was not incorporated as this value was zero for all the stream substances. These coefficients were also used in computation of rate of change of enthalpy per interval.

The algorithm was coded in a PHP platform and the model performance was tested on data collected from three plants. The plants were code named A, B and C. Plant A was a sulphonation processing facility, B a dairy factory and plant C an alcohol distillery. Process descriptions of the plants are shown in Figures 3, 4 and 5 and Tables 1, 2 and 3.



Figure 3. Process flow for oleum production.

The production of oleum, in Plant A, involves heating and cooling. The processes are described in Table 1.

| Stream | Process description |
|--------|-----------------------------------------|
| 1 | Heating of Sulfur |
| 2 | Melting of Sulfur |
| 3 | Further heating of molten sulfur |
| 4 | Heating Regeneration water |
| 5 | Boiling Regeneration Water |
| 6 | Further heating of Regeneration steam |
| 7 | Heating Sulfur lagging water |
| 8 | Boiling Sulfur lagging water |
| 9 | Further heating of Sulfur lagging steam |
| 10 | Process air cooling |
| 11 | Sulfur dioxide cooling |
| 12 | Reactor Stage One Cooling |
| 13 | Reactor Stage Two Cooling |
| 14 | Reactor Stage Three Cooling |
| 15 | First Stage Cooling of Sulfur Trioxide |
| 16 | Second Stage Cooling of Sulfur Trioxide |
| 17 | Removal of Heat of Neutralization |





Figure 4. Process flow for dairy plant.

Table 2 describes the processes involved in the dairy plant.

| Stream | Process description |
|--------|----------------------------------------|
| 1 | Fresh milk cooling |
| 2 | Pasteurization of milk |
| 3 | Cooling of pasteurized milk |
| 4 | Ultra-Heating of Milk |
| 5 | Cooling of Ultra-Heated Milk |
| 6 | Heating of Sterilization Water |
| 7 | Boiling of Sterilization Water |
| 8 | Further Heating of Sterilization Steam |

| Table 2. Proces | s streams | for p | lant B. |
|-----------------|-----------|-------|---------|
|-----------------|-----------|-------|---------|



Figure 5. Process flow for distillery plant.

The heating duty for the distillery plant is in form of steam, used in the distillation column. The cooling duty for the distilled products is supplied using chillers and cooling towers. The distillary process streams are decribed in Table 3.

| Table 3. Process stream for plant (| С. |
|-------------------------------------|----|
|-------------------------------------|----|

| Stream | Process description |
|--------|-----------------------------------------------------------|
| 1 | Fermentation process cooling |
| 2 | First stage wash heating process |
| 3 | First stage wash boiling process |
| 4 | Second stage wash heating process |
| 5 | Second stage wash boiling process |
| 6 | Third stage wash heating process |
| 7 | Third stage wash boiling process |
| 8 | First stage condensation of alcohol vapor (acetaldehyde) |
| 9 | Second stage condensation of alcohol vapor (ethanol) |
| 10 | Third stage condensation of alcohol vapor (fusel alcohol) |
| 11 | Chilling of acetaldehyde |
| 12 | Chilling of ethanol |
| 13 | Chilling of fusel alcohol |

The study collected temperature, mass flow rate, specific heat capacities, polynomial temperature coefficients of specific heat capacities and ΔT_{min} specific to streams, per each stream for

the three plants. Stream specific values of ΔT_{min} were obtained from [2] and [6]. Coefficients A, B and C were obtained from [8] and [9].

Heat balancing and energy targeting results from the proposed and the traditional models were compared. For this comparison, the proposed model was denoted as Scenario One and the conventional model was denoted as Scenario Two. Scenario Three and Scenario Four were tested too and they involved use of only one of the suggested improvements on pinch analysis tool. Table 4 shows a summary of these scenarios.

| Scenario | ΔT_{min} Approach used | C _p Approach used | Comments |
|----------|--------------------------------|------------------------------|-------------------------------------|
| One | Stream specific value | Polynomial temperature | This is the model proposed for |
| | | coefficients | adoption |
| Two | Global value | Interpolated values | This is the base model. It is the |
| | | | commonly used model for targeting |
| Three | Global value | Polynomial temperature | This is a variation to the proposed |
| | | coefficients | model |
| Four | Stream specific value | Interpolated values | This is a variation to the proposed |
| | | | model |

Table 4. Description of scenarios.

Scenarios Three and Four were used to assess the effect on energy targets if only one of the suggested improvements was implemented. The two Scenarios do not apply to heat balancing because the process is not affected by ΔT_{min} .

What-if simulations were carried out on some streams from the three plants, to determine the pattern of deviations in cooling and heating duties determined using the Scenarios One and Two.

3. Results and discussion

Results of performance testing of the proposed model are presented in this section. The heat balancing results for Scenario One and Two are presented and analyzed. Energy targeting results for Scenarios One, Two, Three and Four are also presented and analyzed.

3.1. Heat balance

The data collected from plants A, B and C is shown in Tables 5, 6, 7, 8, 9 and 10.

| Stream | Ts (°C) | Tt (°C) | ṁ (kg/s) | ΔTmin | Polynomial Temperature Coefficients of Specific | | | |
|--------|---------|---------|----------|-------|-------------------------------------------------|---------------------------|---------------------------|--|
| No. | | | | (°C) | Heat Capacity | Heat Capacity | | |
| | | | | | A (j/g. °C) | B (j/g. $^{\circ}C^{2}$) | C (j/g. °C ³) | |
| 1 | 33 | 115 | 1.30277 | 15 | 0.73 | 0 | 0 | |
| 2 | 115 | 116 | 1.30277 | 15 | 54 | 0 | 0 | |
| 3 | 116 | 160 | 1.30277 | 15 | 0.73 | 0 | 0 | |
| 4 | 36 | 100 | 0.417 | 5 | 4.02 | 0.58E-3 | 0 | |
| 5 | 100 | 101 | 0.417 | 5 | 2260 | 0 | 0 | |
| 6 | 101 | 163 | 0.417 | 5 | 1.7883 | 1.067E-3 | 0 | |
| 7 | 36 | 100 | 0.417 | 5 | 4.02 | 0.58E-3 | 0 | |
| 8 | 100 | 101 | 0.417 | 5 | 2260 | 0 | 0 | |
| 9 | 101 | 163 | 0.417 | 5 | 1.7883 | 1.067E-3 | 0 | |
| 10 | 201 | 1 | 1.2348 | 5 | 1.03409 | 0.27E-3 | 0 | |
| 11 | 566 | 528 | 0.9933 | 10 | 0.373 | 0.001 | 77E-4 | |
| 12 | 534 | 453 | 0.86388 | 10 | 0.24 | 0.002 | 22E-4 | |
| 13 | 585 | 450 | 0.78889 | 10 | 0.24 | 0.002 | 22E-4 | |
| 14 | 485 | 456 | 0.686700 | 10 | 0.24 | 0.002 | 22E-4 | |
| 15 | 456 | 203 | 0.445698 | 10 | 0.24 | 0.002 | 22E-4 | |
| 16 | 203 | 19 | 0.434509 | 10 | 0.24 | 0.002 | 22E-4 | |
| 17 | 30 | 17 | 0.6678 | 5 | 4.02 | 0.58E-3 | 0 | |

Table 5. Plant A process data used in the proposed model.

Table 6. Plant A process data used in the conventional model.

| Stream No. | Ts (°C) | Tt (°C) | ṁ (kg/s) | 0.5 × ∆Tmin (°C) | Interpolated values of specific heat capacities $(j/g. °C^3)$ |
|------------|---------|---------|----------|---------------------|---------------------------------------------------------------|
| 1 | 33 | 115 | 1.30277 | -5 | 0.73 |
| 2 | 115 | 116 | 1.30277 | -5 | 54 |
| 3 | 116 | 160 | 1.30277 | -5 | 0.73 |
| 4 | 36 | 100 | 0.417 | -5 | 4.18 |
| 5 | 100 | 101 | 0.417 | -5 | 2260 |
| 6 | 101 | 163 | 0.417 | -5 | 2.09 |
| 7 | 36 | 100 | 0.417 | -5 | 4.18 |
| 8 | 100 | 101 | 0.417 | -5 | 2260 |
| 9 | 101 | 163 | 0.417 | -5 | 2.09 |
| 10 | 201 | 1 | 1.2348 | 5 | 1.013 |
| 11 | 566 | 528 | 0.9933 | 5 | 0.82 |
| 12 | 534 | 453 | 0.86388 | 5 | 0.9 |
| 13 | 585 | 450 | 0.78889 | 5 | 0.9 |
| 14 | 485 | 456 | 0.686700 | 5 | 0.9 |
| 15 | 456 | 203 | 0.445698 | 5 | 0.841 |
| 16 | 203 | 19 | 0.434509 | 5 | 0.71 |
| 17 | 30 | 17 | 0.6678 | 5 | 4.18 |

For process plant A, the proposed model used different values of ΔT_{min} per stream and while for the conventional model, a global value of 10 °C was used.

| Stream No. | Ts (°C) | Tt (°C) | ṁ (kg/s) | ∆Tmin (°C) | Polynomial Temperature Coefficients of Specific Heat Capacity | | |
|---------------|---------|---------|----------|------------|------------------------------------------------------------------|---------------------------|--------------------------|
| | | | | | A (j/g. °C) | B (j/g. °C ²) | C j/g. °C ³) |
| 1 | 20 | 3 | 8.61 | 10 | 4.02 | 0.00058 | 0 |
| 2 | 3 | 85 | 8.61 | -10 | 4.02 | 0.00058 | 0 |
| 3 | 85 | 5 | 8.61 | 10 | 4.02 | 0.00058 | 0 |
| 4 | 5 | 147 | 1.87 | -10 | 4.02 | 0.00058 | 0 |
| 5 | 147 | 25 | 1.87 | 10 | 4.02 | 0.00058 | 0 |
| 6 | 25 | 100 | 0.194 | -5 | 4.02 | 0.00058 | 0 |
| 7 | 100 | 101 | 0.194 | -5 | 2260 | 0 | 0 |
| 8 | 101 | 145 | 0.194 | -5 | 1.7883 | 0.001067 | 0 |

Table 7. Plant B process data used in the proposed model.

Table 8. Plant B process data used in the conventional model.

| Stream No. | Ts (°C) | Tt (°C) | ṁ (kg/s) | $0.5 \times \Delta Tmin$ (°C) | Interpolated Values of Specific Heat Capacities $(j/g. °C^3)$ |
|------------|---------|---------|----------|-------------------------------|---------------------------------------------------------------------|
| 1 | 20 | 3 | 8.61 | 2.5 | 4.18 |
| 2 | 3 | 85 | 8.61 | -2.5 | 4.18 |
| 3 | 85 | 5 | 8.61 | 2.5 | 4.18 |
| 4 | 5 | 147 | 1.87 | -2.5 | 4.18 |
| 5 | 147 | 25 | 1.87 | 2.5 | 4.18 |
| 6 | 25 | 100 | 0.194 | -2.5 | 4.18 |
| 7 | 100 | 101 | 0.194 | -2.5 | 2260 |
| 8 | 101 | 145 | 0.194 | -2.5 | 2.09 |

In Plant B, the minimum temperature difference for shifting process temperatures has assumed specific values per stream for the proposed model. For the conventional model, the study used 5 °C.

| Stream No. | Ts (°C) | Tt (°C) | ṁ (kg/s) | ∆Tmin (°C) | Polynomial Temperature Coefficients of Specific Heat Capacity | | efficients of |
|------------|---------|---------|----------|------------|------------------------------------------------------------------|------------|---------------|
| | | | | | A (j/g. °C) | B (j/g. ℃) | C (j/g. °C) |
| 1 | 50.15 | 30.15 | 2.08 | 5 | 4.02 | 0.00058 | 0 |
| 2 | 28.15 | 60.15 | 4.86 | -5 | 3.38 | 0.000488 | 0 |
| 3 | 60.15 | 61.15 | 0.153 | -5 | 586.69 | 0 | 0 |
| 4 | 60.15 | 110.15 | 4.703 | -5 | 3.38 | 0.000488 | 0 |
| 5 | 110.15 | 111.15 | 0.766 | -5 | 837.85 | 0 | 0 |
| 6 | 110.15 | 127.15 | 3.937 | -5 | 3.38 | 0.000488 | 0 |
| 7 | 127.15 | 128.15 | 0.0016 | -5 | 911.9 | 0 | 0 |
| | | | | | | | |

Table 9. Plant C process data used in the proposed model.

Continued on next page

| Stream No. | Ts (°C) | Tt (°C) | ṁ (kg/s) | ∆Tmin (°C) | Polynomial Temperature Coefficients of | | |
|------------|---------|---------|----------|------------|----------------------------------------|-------------|-------------|
| | | | | | Specific Heat | Capacity | |
| | | | | | A (j/g. °C) | B (j/g. °C) | C (j/g. °C) |
| 8 | 61.15 | 60.15 | 0.153 | 2.5 | 586.69 | 0 | 0 |
| 9 | 111.15 | 110.15 | 0.766 | 2.5 | 837.85 | 0 | 0 |
| 10 | 128.15 | 127.15 | 0.0016 | 2.5 | 911.9 | 0 | 0 |
| 11 | 60.15 | 12.15 | 0.153 | 2.5 | 2.031 | 0 | 0 |
| 12 | 110.15 | 11.15 | 0.766 | 2.5 | 2.43 | 0 | 0 |
| 13 | 127.15 | 8.15 | 0.0016 | 2.5 | 2.63 | 0 | 0 |

Table 10. Plant C process data used in the conventional model.

| Stream No. | Ts (°C) | Tt (°C) | ṁ (kg/s) | $0.5 \times \Delta Tmin$ (°C) | Interpolated Values of Specific Heat Capacities (j/g. °C ³) |
|------------|---------|---------|----------|-------------------------------|-------------------------------------------------------------------------------|
| 1 | 323.15 | 303.15 | 2.08 | 5 | 3.514 |
| 2 | 301.15 | 333.15 | 4.86 | -5 | 3.514 |
| 3 | 333.15 | 334.15 | 0.153 | -5 | 586.69 |
| 4 | 333.15 | 383.15 | 4.703 | -5 | 3.514 |
| 5 | 383.15 | 384.15 | 0.766 | -5 | 837.85 |
| 6 | 383.15 | 400.15 | 3.937 | -5 | 3.514 |
| 7 | 400.15 | 401.15 | 0.0016 | -5 | 911.9 |
| 8 | 334.15 | 333.15 | 0.153 | 5 | 586.69 |
| 9 | 384.15 | 383.15 | 0.766 | 5 | 837.85 |
| 10 | 401.15 | 400.15 | 0.0016 | 5 | 911.9 |
| 11 | 333.15 | 285.15 | 0.153 | 5 | 2.031 |
| 12 | 383.15 | 284.15 | 0.766 | 5 | 2.43 |
| 13 | 400.15 | 281.15 | 0.0016 | 5 | 2.63 |

The conventional model in this study used 5 °C for the value of minimum temperature difference.

The heating and cooling loads computed using the proposed and conventional models. The comparisons are as shown in Figures 6 and 7.







Figure 7. Comparison of cooling loads.

Figures 6 reveals that the proposed model has higher heating load values than the conventional model. The percentage differences are 0.33%, 0.66% and 0.73% for plants A, B and C, respectively.

The cooling loads for the two models, shown in Figure 7, revealed mixed results. The proposed model had lower cooling load for plant A, by 21.3%. For plant B, the proposed model had higher cooling load, by 0.40%. There was no difference in the cooling load computed by the two models for plant C.

Further analysis of the behavior of the two models was carried out by simulating heating and cooling loads of selected individual process streams from the three plants. The following streams were selected for heating load simulation:

- i. Main air heater inlet stream
- ii. Heating of Sulfur Lagging Steam
- iii. Heating of Sterilization Steam
- iv. Third Stage Wash Heating ProcessThe following streams were selected for cooling load simulations:
- i. Reactor Stage Two Cooling
- ii. Cooling of Ultra Heated Milk
- iii. Process Air Cooling

An example of the simulation data used to investigate further the behavior of the two models is shown in Table 11.

| | Rate of change of enthe | alpy (kW) | Percentage error |
|-----------------------|-------------------------|--------------|------------------|
| Temperature range (K) | Scenario One | Scenario Two | |
| 369–375 | 5.46 | 5.22 | -4.6 |
| 369–385 | 14.61 | 13.94 | -4.8 |
| 369–395 | 23.8 | 22.66 | -5.03 |
| 369–400 | 28.42 | 27.02 | -5.2 |
| 369–405 | 33.04 | 31.37 | -5.32 |
| 369–410 | 37.68 | 35.73 | -5.46 |
| 369–415 | 42.32 | 40.09 | -5.56 |
| 369–420 | 47 | 44.44 | -5.76 |
| 369–425 | 51.7 | 48.8 | -5.94 |
| 369–431 | 57.26 | 54 | -6.04 |

Table 11. What-if simulation of heating load deviations for the heating of sulfur lagging steam.

From Table 11, the study shows different heating loads when target temperatures are varied from an initial temperature of 369 K.

The simulated heating and cooling loads over different temperature ranges for the proposed and conventional models were presented in Figures 8 and 9, respectively.



Figure 8. Simulation of heating loads over a range of temperatures.



Figure 9. Simulation of cooling loads over a range of temperatures.

The comparisons in Figures 8 and 9 demonstrate that the use of conventional model for cooling and heating load determination can result in either an overestimated or underestimated value, depending on the substance under processing.

For gaseous substances, as illustrated in Figure 8 (a), the conventional model overestimates the required heating and cooling duty, as shown in Figures 9 (a) and (b). For liquid and steam, a reverse behavior is observed, where the conventional model underestimates the required heating and cooling duty. This is shown in Figure 8 (b), (c) and (d) and Figure 3.3 (c).

The magnitudes of the underestimations and overestimations also differ according to the substance under consideration. The percentage deviations are the smallest in liquid substances, ranging from 1.48% to 1.55%, and 1.19% to 1.95%, for wash and milk, respectively.

For steam, the errors are higher compared to liquid. They range between 4.6% to 6.04% and 4.32% to 5.33% for sulfur lagging steam and sterilization steam generation, respectively.

Gases exhibited the highest percentage errors between the models. The errors ranged from 26.38% to 41.25% and 8.88% to 11.47%, for Reactor Stage Two cooling (cooling of SO₂) and Main Air Exhaust (cooling of process air), respectively.

For gaseous substances, the range for SO_2 is higher than the one for air because of the high temperature of the stream. Percentage deviations increase with increase in temperatures. As such, the errors incurred when modeling the loads involving lower temperatures are smaller than those modeled in high temperature are.

3.2. Energy targeting

The targets computed using the proposed model (Scenario One), the conventional model (Scenario Two) and the hybrid of the two models, that is Scenario Three and Four, were presented in Table 12.

| | Internally Recoverable Heat (kW) | | | | | | |
|-------|----------------------------------|--------------|----------------|---------------|--|--|--|
| Plant | Scenario One | Scenario Two | Scenario Three | Scenario Four | | | |
| А | 596.148 | 590 | 480.02 | 530.95 | | | |
| В | 4310.15 | 4123.812 | 4182.315 | 4308.012 | | | |
| С | 1088.36 | 1063.959 | 1094.12 | 1058.52 | | | |

 Table 12. A comparison of energy targets from different models.

The results show that energy targets computed using the proposed model are higher than those computed using the conventional model, Scenario Three and Scenario Four, save for plant C, where the Scenario Three has higher targets. The proposed model has higher targets than the conventional model by 1.03%, 4.5% and 2.2% for plants A, B and C, respectively.

The proposed model has higher targets than Scenario Three model, by 24.1% and 3.05% for plants A and B, respectively, and less targets, by 0.5%, for plant C. Similarly, the proposed model targets are higher than those of Scenario Four, 12.27%, 0.04% and 2.8% for plants A, B and C, respectively.

The findings imply that if the proposed model is used to determine the maximum internally recoverable energy available in a process, more targets can be set. The difference of these targets from those computed using the conventional model vary per plant. Partial modifications to the conventional model, which can be expressed as Scenario Three and Four, also lead to different targets. Both the models record mixed results per plant, with some recording higher targets and others recording lower targets.

4. Conclusions

In pinch analysis, the use of interpolated values of specific heat capacity and global values of ΔT_{min} has been commonly used for heat balancing and energy targeting. These methods are based on approximations. This study attempted to improve the methods by using the polynomial temperature coefficients of specific heat capacities for different substances and stream specific values of ΔT_{min} .

Data from three plants that were used to test the proposed model and compare to the conventional model revealed that the use of the conventional model leads to variations in both heat balancing and energy targeting. When calculating heat balance using the proposed model, the heating and cooling load for liquids was higher for steam and liquids, compared to the conventional model. For gases, this trend was reversed. The loads for the proposed model were lower compared to the conventional model.

Simulation results show that the percentage deviation in the computed loads differed, with higher magnitudes observed in gases and the lowest magnitudes observed in liquids. Deviations arising from the model used to computed loads for liquids ranged from 1.48% to 1.95%. For steam, they ranged from 4.32% to 6.04% while for gases, they ranged from 11.47% to 41.25%. As well, as temperature increases, the deviations increase. At higher temperature, the method used to compute

the loads increased the deviation sensitivity. The temperature variation sensitivities recorded in gaseous substances was higher than that of liquids.

Significant differences were also noted in energy targeting when the proposed method was employed and compared to other models. The conventional model was found to underestimate the internally recoverable heat. The percentage deviations varied with the plant under consideration. For the three plants observed, the deviations varied by 1.03%, 4.5% and 2.2% for A, B and C respectively. The use of the proposed model set higher targets. A plant designed or retrofitted using this energy targeting approach is therefore likely to have low energy operating costs.

The results of this study suggest that the use of the conventional method for heat balancing and energy targeting is susceptible to design errors. For accurate predictions of the maximum internally recoverable heat in a thermochemical plant therefore, it is advisable to use the temperature dependent specific heat capacities and stream specific values of ΔT_{min} . The susceptibility to errors is more pronounced in exchangers that involve gases and processes that have high temperature variations.

This paper suggests recommendations for further studies in this area. First, there is scarce literature on the use of the stream specific values of ΔT_{min} and the polynomial temperature coefficients of mixed substances. These lead to use of approximation methods when selecting the values to use. In order to improve investigation into the model, experiments should be carried out to determine polynomial temperature coefficients of mixed substances.

As well, models on the optimal stream specific values of ΔT_{min} for different substances should be developed. The allowable minimum temperature differences between two fluids exchanging heat depends on the geometry of the exchanger and the overall heat transfer coefficient. In most design cases, these depend on the experience of the designer. This can be improved through development of theoretical models that can help designers select the appropriate values of ΔT_{min} basing on the overall heat transfer coefficients and geometry of the exchangers.

Lastly, it is recommended that more empirical studies be carried out using this proposed approach, on plants that process different products. Studies should be extended beyond the alcohol refinery, sulphonation and dairy products processing plants used in this work. This will be useful in attempting to establish and confirm the trends observed in this study, especially in terms of percentage differences.

Author Contributions

Dr.Eng. Ndiritu and Prof. Kinyua were instrumental in conception and design of this work, and in revising it critically before submission. Fenwicks participated in work design, data collection, drafting the report and carrying out the reviewers' change requests.

Conflict of interest

The authors declare no conflict of interest.

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