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Integration of batch processes is preferably accomplished by indirect heat recovery using thermal energy storage. Such processes may have brief peaks in energy demand, necessitating high storage capacity within short time periods. However, practical space constraints often limit maximal storage volumes, restricting the potential capacity to recover process heat. Consequently, the required utility costs of storage-limited integration solutions are increased, influencing their economic viability. Given increasing importance in the industry to utilize thermal energy efficiently, process operators may want to explore what is maximally possible energetically, within current space constraints, before contemplating expansion and further capital expenditure. Therefore, linear programming is utilized to determine storage integration solutions which maximize heat recovery per batch for volume-limited sensible stratified storage, specified by an insight-based approach from Pinch Analysis. The results produce a process-specific capacity limitation chart of batch-wise maximal heat recovery as a function of limited capacity, allowing generation of optimal storage loading and unloading profiles. Total batch costs (investment and operating cost per batch) are used to estimate the influence of limited capacity. The methodology is demonstrated in a case study. The resulting capacity limitation chart shows that for a stratified storage with four VSUs, which would require a volume of 97.4 m³ to achieve 100% of the indirect heat recovery potential, approximately 60% can be covered by an 8 m³ storage.

1. Introduction

In batch and non-continuous processes, heat can be recovered indirectly through the integration of thermal energy storage (TES). If direct heat recovery (HR) potential is achieved, further heat integration can only take place via indirect HR using intermediate loops (ILs), and TESs also termed as heat recovery loops. Usually, needed storage capacity is determined using a time dependent energy balance of the TES and often optimized in terms of annualized costs (i.e. Atkins et al. 2012). A common form of TES is sensible thermal energy storage (STES), whereby heat is stored by temperature differences between layers of storage media (volume storage units, VSUs). Currently, no work regarding optimization of possible HR under storage volume constraints has been published, representing a gap in the available literature, which is addressed in this paper. A general aim of the work is to enable the finding of smaller storage tanks which can cover the major portion of the possible HR. This causes lower investment costs and saves space. Further interests lie in the management of the operation of such capacity-limited storages.

2. Methodology

A thermodynamic optimization model for maximizing HR for a given storage volume is presented. The optimization assumes pre-specification of the TES, graphically, using the Indirect Source Sink Profile (ISSP) method (Krummenacher, 1991). Information on using ISSP to determine TES VSU temperatures is given by...
Olsen et al. (2016). Although the optimization model presented here uses the ISSP to determine VSU temperature levels, it is also compatible with more sophisticated mathematical methods.

2.1 Thermodynamic optimization model

In Figure 1 the superstructure for STES is given. Subscript $h$ ($1...H$) denotes hot process streams and $c$ ($1...C$) cold process streams. Generally, process streams are indexed with subscript $s$. Subscript $k$ ($1...K$) refers to the IL and also the VSU, whereby the top VSU is $k = K + 1$. Subscript $l$ ($1...L$) represents the current TS.

Figure 1: Superstructure of stratified storage with utility re-balancing HEX on the ILs

$H_h$ and $C_c$ represent hot and cold process streams. $T_h$ and $T_{s,k}$ represent VSU temperature and stream cut-off temperature; both provided by the ISSP. These time independent temperatures appear before and after each process heat exchanger (HEX). $Q_{s,k,l}$ represents heating and cooling of circulated storage mass ($m_{s,k,l}$) by process streams, per stream, IL and TS. $Q_{H,U,c,ISSP}$ and $Q_{C,U,h,ISSP}$ represent the time-independent utility requirements, assuming only vertical heat transfer, given by the ISSP. Process streams excluded due to the ISSP must also be covered by these external utilities. $Q_{H,U,k,l}$ and $Q_{C,U,k,l}$ refer to utility re-balancing, with associated mass transfers $m_{H,U,k,l}$ and $m_{C,U,k,l}$; introduced within each IL to reduce the storage volume.

$M_{k,l}$ represents the mass inventory of each VSU per TS ($l = 0...L$), where $l = 0$ symbolizes initial mass inventory. Generally, mass transfers are time-dependent and change as the storage is loaded or unloaded. For modelling, storage medium density, heat capacity flowrates and film heat transfer coefficients of both streams and storage flows, are all assumed constant throughout operation. Additionally, the stratification of VSUs is considered ideal (no mixing). All heat losses and reversibilities are assumed to be zero. Stream utility demands $Q_{H,U,c,ISSP}$ and $Q_{C,U,h,ISSP}$, are given by:

$$Q_{H,U,c,ISSP} = \Delta t_c C_P c (T_c, T - T_{c,K+1})$$

$$Q_{C,U,h,ISSP} = \Delta t_h C_P h (T_h, T - T_{h,T})$$

where, $\Delta t_c$ and $\Delta t_h$ is the duration, $C_P c$ and $C_P h$ the capacity flow rate, and $T_c, T$ and $T_h, T$ the target temperature, of the cold and hot process stream. Heat supplies and demands $Q_{s,k,l}$ and corresponding transferred mass $m_{s,k,l}$, within each TS are given by:

$$Q_{s,k,l} = \Delta t c C_P c (T_{s,k+1} - T_{s,k})$$

$$m_{s,k,l} = \frac{Q_{s,k,l}}{c_{p sm} (T_{s,k+1} - T_k)}$$
Thereby, $T_{s,k}$ and $T_{s,k+1}$ are the corresponding cut-off temperatures, $c_{p,sm}$ the storage media specific heat capacity, and $\Delta t$ is the TS duration. The VSU mass inventory at the end of each TS, $M_{k,l+1}$, is layer dependent. Eq(5) describes the general mass balance for each intermediate VSU. Eq(6) and Eq(7) describe the mass balance for the bottom and the top VSU.

\begin{equation}
M_{k,l+1} = M_{k,l} + \sum_{c} m_{c,k-1,l} - \sum_{h} m_{h,k,l} - \sum_{c} m_{c,k,l} - m_{mU,k-1,l} - m_{CU,k-1,l} + m_{cu,k,l}
\end{equation}

\begin{equation}
M_{1,l+1} = M_{1,l} - \sum_{h} m_{h,1,l} + \sum_{c} m_{c,1,l} - m_{mU,1,l} + m_{CU,1,l}
\end{equation}

\begin{equation}
M_{k+1,l+1} = M_{k+1,l} + \sum_{h} m_{h,k,l} - \sum_{c} m_{c,k,l} + m_{mU,k,l} - m_{cu,k,l}
\end{equation}

Thereby mass inventories and mass transfers have always to be equal or larger than zero. The needed utility for the re-balancing, $Q_{HU/CU,k}$, is given by:

\begin{equation}
Q_{HU/CU,k} = m_{mU,CU,k} c_{p,sm}(T_{k+1} - T_{k})
\end{equation}

Required HEX areas are defined by Eq(9).

\begin{equation}
A_{HEX} \geq \frac{Q_{HEX,k}}{U_{HEX} \Delta T \Delta t}
\end{equation}

The optimization maximizes possible HR for a given volume, and the objective function is defined by:

\begin{equation}
HR = \max \left( \sum_{h} \sum_{k} \sum_{l} Q_{h,k,l} - \sum_{k} \sum_{l} Q_{CU,k,l} \right) = \max \left( \sum_{c} \sum_{k} \sum_{l} Q_{c,k,l} - \sum_{k} \sum_{l} Q_{HU,k,l} \right)
\end{equation}

Eq(10) includes all heat inputs and outputs, excluding utility rebalancing. Both sides give the same result, as mass inventory at the start and end of a batch cycle have to equate:

\begin{equation}
M_{k,0} = M_{k,L}
\end{equation}

Additionally, the possible range of mass inventories is constrained, whereby $M_{k,max}$ is the maximal mass inventory of each VSU within a batch cycle and is given by.

\begin{equation}
0 \leq M_{k,l} \leq M_{k,max} \leq M_{tot}.
\end{equation}

In stratified storages, the volume of each VSU is not static and is constrained only by total volume as follows:

\begin{equation}
M_{tot} = \sum_{k} M_{k,l=0}
\end{equation}

To solve the optimization problem the open source solver Clp (COIN OR linear programming) which is a simplex algorithm from the optimization suite COIN-OR is used (Loungee-Heimer, 2003).

2.2 Cost model

To determine how limiting storage affects total costs, total batch costs (TBC) are used (Krummenacher, 1991). TBC give costs per batch, accounting for investment costs via a batch-wise annuity factor $a_b$ ($N$ batches; interest $i$ and period $n$) and operating costs $C_{op}$ of all streams. $Q_{HU/CU,k}$ and $C_{HU/CU}$ represent utility costs. Investment costs for HEXs and TESs of size $X$, are estimated by a generalized six-tenths method, for a base cost $C_{inv,b}$, reference size $X_0$ and cost $C_{inv,0}$, with associated degression factor $f_{X}$. 

\begin{equation}
TBC = a_b \sum_{h} c_{inv,h} + C_{op} ; c_{inv,h} = c_{inv,b} + C_{inv,0} \left( \frac{X}{X_0} \right)^{f_X} ; C_{op} = \sum_{h} c_{mU} Q_{HU,k,l} + C_{CU} Q_{CU,k,l}
\end{equation}

\begin{equation}
a_b = \frac{i(1+i)^n}{(1+i)^n - 1}
\end{equation}
3. Illustrative case study: Modified single product batch plant

A three-stage batch process first introduced by Gremouti (1991), and later modified (Eiholzer, 2014), has been selected as the case study. The process comprises two batch reactors and a distillation column. Relevant stream data is shown in Table 1. Table 2 gives the utilized investment cost parameters.

Table 1: Stream data – modified SPBP

<table>
<thead>
<tr>
<th>Stream</th>
<th>$T_{in} , ^\circ C$</th>
<th>$T_{out} , ^\circ C$</th>
<th>CP kW/K</th>
<th>$\Delta h , kW$</th>
<th>$h , W/m^2K$</th>
<th>$t_{u} , h$</th>
<th>$t_{w} , h$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distillcondenser</td>
<td>111</td>
<td>110</td>
<td>403.9</td>
<td>403.9</td>
<td>4,000</td>
<td>3.08</td>
<td>5.25</td>
</tr>
<tr>
<td>Distillsubcool</td>
<td>110</td>
<td>50</td>
<td>0.8</td>
<td>46.2</td>
<td>1,000</td>
<td>3.08</td>
<td>5.25</td>
</tr>
<tr>
<td>Refluxcondenser</td>
<td>135</td>
<td>134</td>
<td>917.7</td>
<td>917.7</td>
<td>2,000</td>
<td>6.33</td>
<td>7.83</td>
</tr>
<tr>
<td>Productcooling 1</td>
<td>140</td>
<td>75</td>
<td>19.4</td>
<td>1,259.4</td>
<td>1,000</td>
<td>7.83</td>
<td>8.50</td>
</tr>
<tr>
<td>Productcooling 2</td>
<td>85</td>
<td>35</td>
<td>17.4</td>
<td>871.8</td>
<td>200</td>
<td>9.00</td>
<td>9.67</td>
</tr>
<tr>
<td>Feed preheat</td>
<td>10</td>
<td>60</td>
<td>24.4</td>
<td>1,222.2</td>
<td>500</td>
<td>0.00</td>
<td>0.50</td>
</tr>
<tr>
<td>Distilleboiler</td>
<td>115</td>
<td>116</td>
<td>905.1</td>
<td>905.1</td>
<td>2,000</td>
<td>3.08</td>
<td>5.25</td>
</tr>
<tr>
<td>Feed B preheat</td>
<td>16</td>
<td>78</td>
<td>22.5</td>
<td>1,419.4</td>
<td>800</td>
<td>5.58</td>
<td>6.08</td>
</tr>
<tr>
<td>Feed C preheat</td>
<td>65</td>
<td>100</td>
<td>6.4</td>
<td>223.1</td>
<td>500</td>
<td>5.68</td>
<td>5.98</td>
</tr>
<tr>
<td>Reactantheating</td>
<td>74</td>
<td>95</td>
<td>35.8</td>
<td>751.6</td>
<td>500</td>
<td>6.08</td>
<td>6.33</td>
</tr>
<tr>
<td>Productreheating</td>
<td>72</td>
<td>88</td>
<td>43.1</td>
<td>688.8</td>
<td>500</td>
<td>8.60</td>
<td>8.90</td>
</tr>
</tbody>
</table>

Table 2: Cost function parameters for Eq.(14)

<table>
<thead>
<tr>
<th>Investment</th>
<th>$C_{inv,b}$ (£)</th>
<th>$C_{inv,0}$ (£)</th>
<th>Ref. dimension</th>
<th>$X_{0}$</th>
<th>$f_{d,X}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HEX</td>
<td>0</td>
<td>40,000</td>
<td>Area (m²)</td>
<td>100</td>
<td>0.78</td>
</tr>
<tr>
<td>TES</td>
<td>0</td>
<td>150,000</td>
<td>Volume (m³)</td>
<td>100</td>
<td>0.71</td>
</tr>
</tbody>
</table>

Utility costs are given as 80 £/MWh (hot) and 5 £/MWh (cold). Storage media costs (water) are assumed negligible. Batch-wise annuity factor is calculated for a 5 y period at 10 % interest for 2,000 batches/y.

4. Results and discussion

The STES is first defined using the ISSP (Figure 2a) which allows exploration of trade-offs between VSU numbers (black dots), their operating temperatures, and HR (black lines; enthalpy span indicates HR within IL).

Figure 2: (a) ISSP of the SPBP with HR = 2.9 MWh per SROP for SROP. (b) Loading/unloading profile of a 3-IL STES.

As only VSU temperatures and HR are defined explicitly using the ISSP, storage sizing is completed by mass and energy balancing within each TS. The shaded grey area represents an area of design freedom, termed an “assignment zone”, within which VSU operating temperature can be chosen by graphical placement. Placement also defines the enthalpy ranges of neighboring ILs. Zone generation is done algorithmically, to
minimize the number of VSUs for a given HR. HR of 2.9 MWh allowed an adequate trade-off between HR, and IL number liked to system complexity; the maximum amount of HR for a STES comprising four VSUs. The VSU operating temperatures have been chosen according to minimizing the number of process streams which are connected to more than one IL, which minimizes the number of HEXs required and the complexity of the system. High temperature differences between VSUs facilitate smaller storage volumes. For the top IL, which transfers energy between condensation and vaporization, a smaller temperature difference is allowed. Figure 2b shows the loading and unloading profile of the unlimited storage, as defined by the ISSP. This profile shows how TES inventory is partitioned between individual VSUs during operation. As the TES is loaded, fluid from cooler layers is heated within an IL and passed to hotter layers. In doing so, VSU volumes of hotter layers will grow at the expense of cooler layers. The reverse is true during unloading. Over a stream-wise repeated operating period (SROP), VSU volumes must eventually return to their initial partitioning, to begin the loading cycle again.

During optimization, total storage volume was increasingly limited from the unlimited case (97.4 m³ for 2.9 MWh) to zero volume. The results of the optimization for maximizing HR under these conditions are shown (Figure 3a). The plot shows how total HR (indirect HR of all ILs plus direct HR) reduces as the capacity of the storage decreased, and is termed the Capacity Limitation Chart. The plotted black line shows to what extent indirect HR could be maximized for each limited volume, by the optimization model. In general, as maximum volume is reduced, total HR is decreased from the maximum, to that provided only through direct HR.

It can be observed that maximum HR per SROP, as determined by optimization, transitions through three phases of behavior. As volume is increasingly limited, the loading and unloading profiles of the storage will also change. At any interstitial volume limitation, the loading and unloading profiles can be generated. Figure 3b shows the storage profile when limited to a total volume of 40 m³, marked by the green dot (Figure 3a). In comparison to the unlimited profiles, relative partitioning of the VSU volumes depends on the degree of storage limitation. The profiles are generated using a strategy, whereby VSU are only allowed to empty at the end of a TS, achieved by modulating the flow of storage media within each IL. As a result, the loading and unloading rates of the VSUs (slopes in Figure 3b) and maximal volume per VSU are changed. The smaller mass and heat flows within each TS results in smaller required IL HEXs.

Slope differences in the black line (Figure 3a), indicate two critical changes in how effective the STES system is recovering heat under limitation. Since optimization always reduces the VSUs first, which reduces capacity least (smaller temperature differences between VSUs result in less capacity), two slope changes of the HR curve occur whenever a new VSU becomes empty and cannot be refilled. The two located points are at 18 m³ and 8 m³. The initial limitation from maximal volume to 18 m³ reduces HR approximately 887 kWh. From 18 m³ to 8 m³ HR loss is 239 kWh. Limitation to 0 m³ causes a further 915 kWh HR loss, which is more than reducing from maximum to 18 m³. Throughout limitation, direct HR is constant at 944 kWh. A storage with a volume of just 8 m³ nearly doubles the possible HR to 1,859 kWh. A further increasing of the volume to the
maximal needed volume of 97.4 m$^3$ causes an additional HR of 1,125 kWh. Consequently, 60 % of the total maximum HR can already be achieved within the initial 8 m$^2$, with total HR severely reducing below this limit, representing a minimum recommended volume target of the storage.

Table 3: Costs of SPBP TES under fully limited, partially limited and unlimited conditions

<table>
<thead>
<tr>
<th>Volume (m$^3$)</th>
<th>HR (kWh)</th>
<th>HR relative (%)</th>
<th>$a_b, C_{inv}$ (£/SRP)</th>
<th>$C_{op}$ (£/SRP)</th>
<th>TBC (£/SRP)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>944</td>
<td>32.55</td>
<td>58.12</td>
<td>243.59</td>
<td>301.71</td>
</tr>
<tr>
<td>8.0</td>
<td>1,748</td>
<td>60.28</td>
<td>58.35</td>
<td>170.00</td>
<td>228.35</td>
</tr>
<tr>
<td>97.4</td>
<td>2,900</td>
<td>100.00</td>
<td>69.97</td>
<td>74.95</td>
<td>144.92</td>
</tr>
</tbody>
</table>

As expected TBC were found to be minimum when the storage volume is unlimited (Table 3). Nevertheless, it can be seen that TBC are increased nearly by the same amount by removing an 8 m$^3$ storage or limiting the storage volume to 8 m$^3$. For TBC, operating cost per batch are the dominant contributor. Investment costs affect TBC relatively less, as these are distributed across batches. However, when the volume is limited, two possibilities emerge: Either, storage volume can be kept limited, or space extensions can be considered. Costs for building extensions are not considered in the TBC. By considering these costs, it may be more economical to reduce storage volume.

The optimized arrangement and desired loading/unloading profiles present a potentially challenging control problem, as during operation constant inlet temperatures to the storage are required to prevent severe degradation of the stratified thermocline. Therefore, HEX control strategies should also be considered in future research. Additionally, although HR was maximized, TBC are not minimized under the condition of maximized HR (Krummenacher, 1991). Optimized TBC would allow a better exploration of the trade-offs between HR and relaxing space constraints, provided localized space costs are known.

5. Conclusions

The model maximizes total HR within a process utilizing a HEN and TES, under limited volume conditions. The Capacity Limitation Chart directly shows the relationship between HR and storage volume constraints, demonstrating how detrimental storage volume constraints are to potential future energy savings. It identifies critical storage volumes, where the HR-storage volume relationship critically changes and indicates the minimum recommended storage volume sizes. For the given case study, using the optimization model to locate an arrangement of VSUs and loading profiles, a minimum recommended storage volume of 8 m$^3$ was identified, which could still provide 60 % of the available HR potential.

By adding an economic optimization it could be indicated when relaxing space constraints by further capital expenditure would be appropriate. Where only energy savings are prioritized or no space extension of the plant is possible, the linear programming approach as presented is adequate to perform the optimization.

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