Research Article

Fluid Selection of Organic Rankine Cycle Using Decision Making Approach

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1. Introduction

It is well known that grade of thermal energy is a function of temperature and thus its efficiency in general for power production is variable. However, cheap and easy availability of fuels and large scale economy of the infrastructure compared to alternate sources of energy make it inevitable to choose thermal over any other form of power. Nevertheless, thermal energy possesses variable irreversibility and any system designed to run on it may have a low efficiency, with most of the input heat being wasted at sink temperatures, occasionally going as high as 40% to 60%. Thus, methods must be employed to convert this enormous amount of waste heat energy into useful form. One of the ways of harvesting this energy is to make use of organic rankine cycle (ORC) to produce electricity. ORC is a method of using thermal rankine cycle with organic (low boiling point) fluids to generate electricity from low grade heat energy [1–4]. ORC generally works in the range of temperatures 80 to 350°C but this is not a fixed operating range. ORC is based on the fact that most of the primary thermal sinks used in industry or power production have temperatures that are substantially higher than ambient. These sinks can be used as boilers for the ORC to provide heat to the working fluid which can later be discharged at much lower temperatures. Thereby, it serves the double purpose of producing power and reducing the thermal pollution [5–10].

However, the efficiency of any thermal cycle, including ORC, largely depends upon the properties of the working fluid used [11–13]. Thus, fluid selection forms a critical part of the design process of an ORC based power plant. Fluid properties can largely affect the nature and number of auxiliaries (accessories) that are to be installed for smooth running of the power plant. For example dry fluids require a smaller size of condenser than their wet counterparts and do not require a superheater. Additionally, turbine work and overall efficiencies are a function of fluid properties. Apart from thermal properties, environmental effects need to be considered as well. Therefore, fluid selection for ORC is essentially a multidimensional problem. Additionally, the existence of a large number of plausible candidates makes it a cumbersome task for the engineers to select a suitable fluid. Such multidimensional problems can be solved by two approaches, namely, multiobjective decision making (MODM) and multiattribute decision making (MADM) techniques. MODM makes use of figures of merit, based on functional relation between the various control parameters, to screen and rank the possible candidates [14]. Contrastingly, MADM methods generally compare the different candidate materials based on predetermined mathematical algorithms,
which are used to analyse the desirability of the alternative based on its attributes [15].

Through this paper, an attempt has been made to compare and rank possible fluids for ORC using technique for order preference by similarity to ideal solution (TOPSIS), an MADM method [15–18]. The weights of the different attributes have been calculated using modified digital Logic (MDL) [19]. Dendrogram [20–22], a hierarchical clustering technique, has been used to group and classify the different candidate fluids selected for study. Finally, pearson’s correlation was applied to the properties under study to observe any relevant trend that may exist in the associated properties [23].

2. Materials and Methods

2.1. Materials. Organic Rankine cycle based power plants employ volatile, low boiling point fluids that make use of low temperature waste heat energy for phase change. Generally, chlorofluorocarbons (CFC) possess all the desirable traits required for ORC. However, due to their polluting characteristics they are mostly outlawed. However, for the sake of performance comparison with present alternate fluids their inclusion becomes necessary. There is an impending need to discover fluids which are comparable in performance to the CFCs but are environment friendly. A list of potential candidates chosen for the study is given in Table 1 [1, 24]. The thermal and physical properties relevant to the study are molecular weight (Mol. Wt.), critical temperature (Tc), critical pressure (Pc), specific heat (Cp), capacity, latent heat of vaporisation (L), and dS/dT. The environmental factors considered for this study are atmospheric life (Atm. Life), global warming potential (GWP), and ozone depletion potential (ODP). The temperature of the waste heat is essentially a determining criterion for the grade of energy available for operation of ORC based plant. In this regard, fluids with a low boiling and high critical temperature are essential for high efficiency during continuous working. If the critical temperature of the fluid is far below 300 K, the fluid becomes incapable of rejecting heat to the ambient. Thus, a constraint of \( T_c \geq 300 \text{K} \) was imposed while selecting fluids for the present analysis.

2.2. Modified Digital Logic Approach. Modified digital logic (MDL) is a technique that has been derived from digital logic technique (DL) and was first proposed by Dehghan-Manshadi et al. [19]. Digital logic is used to calculate weights based on the relevant importance of one attribute over the other. It works by comparing two attributes at a time and deciding which one is more important than the other. The total number of possible decisions or outcomes for a given alternative is given by the formula \( N(N - 1)/2 \), where \( N \) represents the number of alternatives under study. In case of a positive response (more importance) “1” is assigned to that particular outcome; else “0” is assigned. The weights are determined by dividing the number of positive decisions by the total number of possible decisions.

Digital logic has certain drawbacks associated with its applicability to the general regime of decision making. In DL there are only two possible outcomes of a decision, which are either less important or more important. This might not be the case as at times the decision maker may feel that the two attributes may be of equal importance. Thus, in MDL this drawback is overcome by using three possible outcomes. In MDL instead of using “1” and “0”, we use three different outcomes which are less important (assign 1), equally important (assign 2), and more important (assign 3). The weights are determined by dividing the number of outcomes for a particular attribute by the total number of outcomes for the logical matrix. For example, in a matrix with three alternatives “a”, “b”, and “c” the order of importance is \( a > b > c \). The total number of possible outcomes is 3. The number of positive outcomes for “a” is 6 since it gets 3 each when compared to “b” and “c”. Similarly, for “b” the number of positive outcomes is 4 as it is more important than “c” but less important than “a”. Finally, the positive outcomes for “c” are 2. Therefore, the total outcomes is sum of all outcomes (=12) and the respective weights are “a” = 0.5, “b” = 0.3333, and “c” = 0.1667. The outcomes and weights for collective properties and then with environmental factor excluded are given in Tables 2 and 3 respectively.

2.3. Multiattribute Decision Making Approach. MADM is one of the two methods that make up the multicriteria decision making [25]. MADM techniques are also sometimes referred to as unsupervised as they do not require a functional relationship to be established between the considered attributes to work. MADM are generally based on predetermined mathematical models and ranking algorithms. On the other hand multiobjective decision making (MODM) uses functional relationship between the different properties to create figures of merit which are used to compare and rank different candidates. Hence, it is also referred to as supervised technique. Here, a MADM method, namely, technique for order preference by similarity to ideal solution is used to rank and compare the different candidate fluids. TOPSIS was first proposed by Hwang and Yoon [15]. TOPSIS is a very popular MADM technique and has been used in various instances to solve many multidimensional engineering and design problems [16–18]. TOPSIS implies that the solution space is a multidimensional hyper plane where the number of dimensions is given by the number of attributes associated with the decision matrix. There are two hypothetical solutions associated with TOPSIS; these are positive ideal solution, and negative ideal solution. Positive ideal solution is the collection of each of the most desirable attributes from the decision matrix; conversely negative ideal solution contains each of the least desirable attributes from the decision matrix. Together these form the two extreme ends of the solution space. The best candidate is one which has the most distance from the negative ideal solution and the least distance from the positive ideal solution (Figure 1).

The TOPSIS method involves the following steps.

Step 1. Construction of normalised decision matrix:

$$r_{ij} = \frac{a_{ij}}{\sqrt{\sum_{l=1}^{m} (a_{lj})^2}}, \quad \forall j,$$

(1)
<table>
<thead>
<tr>
<th>SHARAE number</th>
<th>Name</th>
<th>Mol. Wt.</th>
<th>$T_c$ (K)</th>
<th>$P_c$ (MPa)</th>
<th>$C_p$ (J/(kg·K))</th>
<th>$L$ (KJ/kg)</th>
<th>$dS/dT$ (J/kg·K²)</th>
<th>Atm. life (yrs)</th>
<th>GWP</th>
<th>ODP</th>
<th>TOPSIS index (environmental)</th>
<th>Ranks (environmental)</th>
<th>TOPSIS index (thermal)</th>
<th>Ranks (thermal)</th>
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</thead>
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<tr>
<td>Properties</td>
<td>Number of possible decisions</td>
<td>Number of positive decisions</td>
<td>Weighing factors</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td>0.104167</td>
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<td></td>
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<td></td>
</tr>
<tr>
<td>$T_c$</td>
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<td>22</td>
<td>0.152778</td>
<td></td>
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<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$P_c$</td>
<td>3 2 3 3 3 3 3 3 3 3</td>
<td>22</td>
<td>0.152778</td>
<td></td>
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<td></td>
</tr>
<tr>
<td>$C_p$</td>
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<td>18</td>
<td>0.125</td>
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<td></td>
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<td></td>
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</tr>
<tr>
<td>$L$</td>
<td>3 3 3 3 3 3 3 3 3 3</td>
<td>22</td>
<td>0.152778</td>
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<td></td>
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<tr>
<td>$dS/dT$</td>
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<td>9</td>
<td>0.0625</td>
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<tr>
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<tr>
<td>ODP</td>
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<td>14</td>
<td>0.097222</td>
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<td></td>
<td></td>
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Table 2: MDL weights for collective properties.
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<th>3</th>
<th>4</th>
<th>5</th>
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<th>10</th>
<th>11</th>
<th>12</th>
<th>13</th>
<th>14</th>
<th>15</th>
<th>Number of positive decisions</th>
<th>Weighing factors</th>
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</thead>
<tbody>
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<td>1</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
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<td>3</td>
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<td>2</td>
<td>3</td>
<td>2</td>
<td>3</td>
<td></td>
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<td>3</td>
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<td>1</td>
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<td>1</td>
<td>1</td>
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<td></td>
<td></td>
<td>13</td>
<td>0.216667</td>
</tr>
<tr>
<td>$dS/dT$</td>
<td>2</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td>6</td>
<td>0.1</td>
</tr>
</tbody>
</table>
Figure 1 shows the physical representation of a two-dimensional TOPSIS solution.

2.4. Hierarchical Clustering. Clustering is basically trying to group together different alternatives based on the degree of closeness or similarity between the physical value of their attributes and properties [20, 21]. Dendrogram is a hierarchical clustering technique which can be used to visually represent clusters of multidimensional data [16–18]. Clustering is also an important supplement to any ranking algorithm where it allows the designer or engineer to select the physically closest substitute to an existing alternative where the use or replacement for ultimate optimum may impose several restrictions. Visualisation of a multidimensional space is restricted to a maximum of three dimensions only. While the best visualisation can be made in two dimensions, the upper limit of human observation is three dimensions with the complexity of representation increasing with the number of dimensions. Thus, dendrogram is used to visually represent multidimensional data in two dimensional spaces with y-axis representing the average separation between two or more clusters. This way visual observations can be made of multiattributed data for more than three dimensions. Cophenetic coefficient is used to evaluate a dendrogram’s accuracy in representing the clusters when compared to actual physical parameters. Generally a value of 0.95 or higher is considered to be safely accurate. A dendrogram makes use of Euclidean distance for grouping together clusters of data. The steps involved are as follows.

Step 1. Calculation of Euclidean distance between all the alternatives:

\[
d_{i1 \rightarrow i2} = \left\{ \sum_{j=1}^{n} (V_{ij} - V_{2j}) \right\}^{1/2}, \quad \forall j; \forall i. \tag{6}
\]

Step 2. Determination of distance matrix is done as:

\[
D = [d_{ij}]_{m \times m}, \tag{7}
\]

where \(D\) is a square matrix consisting of Euclidean distances of \(m\) alternatives, with all its diagonal elements being zero. Now the two alternatives having the least distance will be grouped into a single cluster.

Step 3. Redetermination of distance matrix:

\[
D_1 = [d_{ij}]_{(m-1) \times (m-1)}^{\text{square}} \tag{8}
\]

where \(D_1\) is the revised matrix treating the cluster of first two elements as a single entity. The secondary cluster is determined using the following formula:

\[
d_{(i1,i2) \rightarrow i3} = F_m\left(d_{i1 \rightarrow i3}, d_{i2 \rightarrow i3}\right), \tag{9}
\]

where “\(F_m\)” is the distance relationship determined by the type of linkage used. It is (a) minimum for single linkage, (b) maximum for complete linkage, (c) average for average linkage, and (d) centroidal mean for centroid linkage.
Step 3 is repeated \((m - 1)\) times so that all the alternatives can be grouped into one cluster.

Dendrograms may be formed by using various linkage methods which are used to determine the distance between clusters.

2.5. Pearson's Correlation Coefficient. In order to throw some light on statistical relation between the physical properties under study, correlation coefficient may be calculated. It is the degree of dependence between two variables and is used to predict the general statistical trend that may exist between the properties when compared two at a time. Here we make use of Pearson correlation coefficient \((R)\). It is calculated according to the following formula [23]:

\[
R = \frac{\sum_i (x_{i1} - \bar{x}_{i1})(x_{i2} - \bar{x}_{i2})}{\sqrt{\sum_i (x_{i1} - \bar{x}_{i1})^2} \sqrt{\sum_i (x_{i2} - \bar{x}_{i2})^2}}.
\]

where \(x_{i1}\) and \(x_{i2}\) represent two attributes. The degree of dependence between two variables can be between +1 and –1. Positive correlation indicates simultaneous increase in variable values. However negative correlation indicates opposite behavior among the variables; that is, increase in one variable indicates decrease in other variable. It is to be noted that correlation does not equal causation. Correlated variables indicate that if one variable changes, the other correlated variable changes in a predictable way.

3. Results and Discussions

The desirable properties for an ORC are high: molecular weight, critical temperature, critical pressure, latent heat of vaporization, and \(dS/dT\) slope value, to avoid the use of superheater and reduce the size of condenser required in the power plant. While a low value of specific heat capacity, global warming potential, ozone depletion potential, and atmospheric life is preferred property for a fluid to have low environmental impact. Based on the above criteria the positive (best) and negative (worst) ideal vectors have been calculated for the TOPSIS approach. Finally, the Euclidean distances between the individual attributes of the respective fluids were calculated and added to obtain their distance from the ideal solutions. The ratio of the distances thus obtained is used to determine the ranks. Two separate cases were investigated, with the first being with the consideration of environmental factors (atmospheric life, GWP, and ODP) and the second case being while omitting the afore-mentioned factors. The two cases are compared on ranking schemes to see whether the addition of atmospheric considerations affects the choice of thermally superior fluids.

The first case being investigated is that based on collective properties; that is, environmental properties are included in the study. Ranks of the fluids based on collective and thermal properties are given in Table 1. Even though it can be observed that the top slots have been acquired by CFCs and HFCs, these are of little technological importance as they pose a serious threat to the environment and, hence, their use has been outlawed. However, complete results indicate that R601 (pentane) is the only non-FC fluid that acquires a considerably high rank in both analyses. Also, its rank does not vary much under the two different analyses indicating that not only it is thermally superior but also it is a clean fluid. It is closely followed by butane, cyclopropane, and isobutane which also show high potential as clean and efficient organic fluids. We also come across the observation that under thermal analysis CFCs have obtained higher rankings, but under collective attributes many CFCs have been ranked lower. This is clearly an indication that when evaluated on a combined basis, CFCs rank inferior in performance when compared to their organic counterparts. The organic fluids do not suffer from drastic fall in their ranks indicating an overall optimum performance characteristic as thermally superior and non-polluting.

The second analysis was done by excluding the environmental properties. The TOPSIS indices and ranks for the second analysis are given in Table 1, columns 14 and 15, respectively. The general trend of ranking is observed to favour CFCs indicating their superior performance in thermal cycles. The main reason behind their phase out was their highly polluting nature which is clear by the huge rank difference displayed by CFCs when ranked on a collective basis. It is also observed that under the consideration of environmental factors rank compromise is severe for CFCs relative to organic fluids.

The respective weights of the different attributes using MDL for the first and second analysis are given in Tables 2 and 3, respectively. These weights are based on authors' opinion and are open to discussion. It can be observed that for combined properties \(T_r\), \(P_r\), and \(L\) receive the highest and equal weights of (0.15), followed by specific heat capacity (0.125) and molecular weight (0.10) which is used to determine the density of the fluids. The least weight is assigned to slope \(dS/dT\) (0.06), the respective weights of the properties determine their order of importance. While for the second analysis the highest and equal weights are again assigned to \(T_r\), \(P_r\), and \(L\) being 0.21, followed by \(C_p\) having a weight of 0.15. Here the least and equal weight is assigned to molecular weight and \(dS/dT\) indicating their lower significance in the choice for selection of fluids.

Finally in order to supplement the ranking and to visualise the clustering effect that properties have on the fluids, two separate dendrograms are prepared. A physical representation of a two-dimensional clustering for six alternatives is illustrated in Figure 2. The clusters are formed based on the minimum distance that exists between (a) two alternatives \([a-b; c-d]\), (b) two clusters \([ab];[cd]\), and (c) alternative and a cluster \([ab];[cd]\). It is to be noted here that the only factor relevant to the clustering is the magnitude of physical distance. Hence, physical similarity is expected from the members of a cluster with deviation increasing with the increases in average distance (of separation). Figure 2 can also be used to explain the anomaly that exists between ranking and clustering algorithms. Though the alternatives “e” and “f” may differ largely in ranks based on their attributes, the average distance (of separation) for both of them will differ by a small amount only.
The colouring scheme of the dendrograms created is as follows: red indicates a CFC/HFC, green indicates an organic compound, blue indicates an inorganic compound, and black colour has been used to indicate an anomalous pairing. Dendrogram for the first and second analysis can be seen in Figures 3 and 4, respectively. It may be clearly observed from Figure 3 that there is high order of correlation among the organic fluids, which form a very ordered cluster, with the exception of 8 which is a CFC. Ethane, however, shows deviating behaviour as it is not closely clustered with the rest of the organic compounds. Low degree of separation also indicates that they are expected to display similar performance, which is expected from closely grouped alternatives. It can be seen from Figure 3 that the average separation changes when only thermal properties are included for the clustering algorithm. This indicates that when polluting effects are excluded there is a large variation between the expected performances of the fluids. The cophenetic coefficient for both the dendrograms was found to be more than 0.90 thereby signifying that dendrogram is safely accurate.

The calculated values of Pearson’s correlation coefficients between different attributes are mentioned in Table 4. High degree of correlation has been depicted in bold. These correlation coefficients may be useful for data-mining purposes, trend prediction, and critical analysis of performance of different fluids compared to the variation in different properties.

A similar type of study involving selection of working fluid for organic Rankine cycle has been done by Handayani et al. [26]. However, it is limited to a low number of working fluids. The present study, however, deals with a large number of organic and inorganic working fluids. Hence, it is a more comprehensive approach. Additionally, the present study uses MDL approach for weight determination. Finally, correlation between their properties has been discussed which will help to discern their behaviour under different working environments.

4. Conclusion

In this paper MADM method has been employed for selection of optimum working fluid for organic Rankine cycle. TOPSIS approach is used to rank ORC fluids with and without consideration of environmental factors. Subjective weights have been calculated for the analysis using modified digital logic approach. In both the cases it is observed that pentane shows promising results as the only dry organic liquid to obtain top slots in both the ranking procedures.
Table 4: Pearson’s correlation coefficients.

<table>
<thead>
<tr>
<th>Properties</th>
<th>Mol. Wt.</th>
<th>$T_c$</th>
<th>$P_c$</th>
<th>$C_p$</th>
<th>$L$</th>
<th>$dS/dT$</th>
<th>Atm. Life</th>
<th>GWP</th>
<th>ODP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mol. Wt.</td>
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<td>-0.0424</td>
<td>-0.5299</td>
<td>-0.5329</td>
<td>-0.4785</td>
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Further investigation is warranted for the use of pentane as a suitable working fluid for the organic rankine cycle power generation through recovery of low grade heat energy. Well-defined clustering is observed for organic fluids indicating exhibition of generalised behaviour among them which is likely to promote interchangeability.

The results of the present study are in good agreement with earlier studies of similar nature. Thus, it confirms the fact that decision making theories may be successfully applied to fluid selection problems for thermal power generation cycles.

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References


