SYSTEM MODELLING FOR RANKINE CYCLE WASTE HEAT RECOVERY FROM A SPARK IGNITION ENGINE

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ABSTRACT
The Rankine Cycle can be used to convert low grade heat, including the dual heat sources of a spark ignition engine, into useful energy. To maximise the shaft power output, by optimising the capture of waste heat, requires detailed consideration of the cycle thermodynamics. A spreadsheet model for each proposed Rankine Cycle configuration has been developed and the results verified by comparison with a standard industry process engineering software package. The spreadsheet model results may be more reliable because the thermodynamic data are based on real data rather than equations of state. Comparisons of the proposed cycles are given for hexane as the working fluid.

INTRODUCTION
Waste heat recovery from a spark ignition generator is a means of increasing its overall efficiency and viability for distributed generation. The Rankine Cycle is a heat engine capable of being used as a bottoming cycle to convert low grade heat into useful work and ultimately electricity. Increasing the overall efficiency of the generator will result in lower greenhouse gas emissions per unit of electricity produced.

Although there is considerable interest in the Rankine Cycle for waste heat, solar thermal and geothermal applications, the heat considered is normally from a single source. A small spark ignition generator, suitable for commercial distributed generation applications, has two heat streams that are potential heat sources for the Rankine Cycle. These two heat streams are the engine coolant and exhaust. Both heat streams are generally considered to contain similar quantities of heat, albeit with very different qualities. The challenge is to maximise the shaft power output by optimising the total heat utilisation from both these heat sources in a cost-effective manner.

In this work, a number of Rankine Cycle configurations were proposed to utilise heat from the coolant and exhaust of a spark ignition engine from a generator. The tools to perform the required optimisation techniques are not built into commercial process engineering software packages such as HYSYS. In order to solve, evaluate and compare the cycle configurations, a spreadsheet model for each was developed. Each spreadsheet model was designed to maximise the shaft power output from the Rankine Cycle, by optimising the total heat utilisation. This meant there was more interest in the overall system heat to shaft power conversion efficiency than the cycle efficiency.

This paper describes the general optimisation procedure, underlying assumptions and variables for each of the different cycles. Selected key outputs and results are compared to a commercial process engineering software package, HYSYS (an ASPEN product). Comparisons of the cycle results are also made for hexane.

THERMODYNAMICS OF RANKINE CYCLES
The ability to exploit waste heat using the Rankine Cycle depends upon the fluid and configuration of the cycle. A basic Rankine Cycle involves circulation of a volatile working fluid. Heat is used to vaporise the liquid working fluid into a high pressure vapour. The vapour passes through an expander to create useful mechanical work. The cycle is completed by condensing the vapour back to a liquid and pumping it through the heat source again. The significant thermodynamic points within the cycle are:
1. The high pressure liquid working fluid leaving the pump
2. The hot high pressure vapour entering the expander
3. The warm, low pressure expanded vapour leaving the expander
4. The low pressure condensed working fluid entering the pump.

Maximising the heat to mechanical energy conversion in a Rankine Cycle requires optimising the available heat capture in the working fluid and maximising its isentropic expansion across the expander. This work also assumes that the temperature of the heat sink is constant.
The amount of heat that can be captured from a heat source is limited by the temperature at which the working fluid begins to boil. Heat transfer requires the temperature of the heat source to remain above that of the working fluid. The minimum temperature difference occurs at the pinch point and is called the approach temperature, Figure 1. In designing a Rankine Cycle, the minimum approach temperature needs to be specified and this normally 5 or 10°C. “The best efficiency and highest power output is usually obtained when the working fluid temperature profile can match the temperature profile of the heat source” [1]. This is illustrated in Figure 1 where the specific heat of vaporisation of an organic fluid, R114, is lower than water and follows the temperature profile of a gas turbine exhaust better [2].

**MODELLING APPROACH**

The approach to modelling each Rankine Cycle configuration was to develop a spreadsheet model that solved sequential equations relatively easily and accurately. The model considered each significant point in the Rankine Cycle and then balanced the heat and mass flow properties to maximise the shaft power output for the available heat. Some properties of the significant points were defined by the heat source, while others arose from the assumptions and constraints, and the rest were calculated by solving the heat and mass balance equations. The spreadsheet was linked to the NIST “Reference Fluid Thermodynamic and Transport Properties” database “REFPROP” [4] to allow direct access and determination of the fluid thermodynamic properties for each significant point.

The general optimisation procedure and underlying assumptions are described below. Further constraints for each cycle are also described in the Cycle Details.

**Model Optimisation Procedure**

The model optimisation procedure was designed to solve the heat and mass balance equations. This was achieved in Microsoft Excel using its in-built Solver optimisation routines that optimises the value of a target cell, based on the formula in the target cell, by changing the values in adjustable cells and applying other constraints put on the system. For non-linear problems, the MS Excel Solver uses a generalised reduced gradient (GRG2) optimisation procedure [3]. For linear and integer problems, the simplex method, with bounds on the variables, and the branch-and-bound method are used [5].

The generic sequence of calculations was:

i) Condenser temperature determines the thermodynamic properties of the pump feed and as the fluid is a saturated liquid, the vapour pressure can be calculated. Once the pressure and temperature are known, enthalpy, entropy and density can be calculated via the NIST REFPROP equation of state.

ii) The temperature at which the fluid boils determines the expander inlet pressure of the system via the saturated vapour pressure. This pressure is used to determine the dP across the pump. For simplification the pump is assumed to be 100% efficient, therefore there is no entropy change across the pump. With the outlet pressure and entropy accounted for, the temperature, enthalpy and entropy are calculated.

iii) The pressure of the expander inlet has been calculated in step (ii). The temperature and superheat of the fluid is determined by the cycle design. In the simple cycle case, the working fluid is saturated and hence the pressure and temperature are defined.

iv) The mass flow is determined by balancing heat in and working fluid enthalpy change. “Heat in” is the available heat source. The change in enthalpy of the working fluid is the sum of sensible and latent heat, multiplied by the mass flow. Where the expander inlet pressure and temperature are known, this is a simple back calculation. However if the temperature and pressure are not fixed, as in the High Temperature Saturated Simple Cycle, then iteration is required to balance the heat in and working fluid change in enthalpy. The superheat and boiler temperature are simultaneously adjusted to maximise the expander power by the solver optimisation routine.

![Figure 1. Comparison of temperature profiles and pinch points for a gas turbine exhaust and water (left) and R114 (right) working fluids](image-url)
v) The expander power calculation is based on an isentropic expansion of the working fluid. The spreadsheet first calculates an ideal (constant entropy) expansion, then applies the expander efficiency to obtain the real expansion result.

vi) If a recuperator is used in the cycle then the model checks to see if there is any heat available. This will depend on the outlet temperature of the expander, the condenser temperature and the minimum approach temperatures (10°C).

Assumptions
The underlying assumptions in the modelling have been:
- The outlet of the condenser has a temperature of 50°C, which dictates the minimum pressure of the cycle
- An expander isentropic efficiency of 70%
- Maximum pressure ratio, i.e. the ratio of expander outlet pressure relative to the inlet pressure, of 20
- No heat losses or parasitic power i.e. for the working fluid pump or condensing system, which could be significant and vary for each cycle and fluid
- Available coolant heat of 25 kW, assumed to be cooled from 90 to 85°C
- Available exhaust heat of 17.3 kW by cooling from 520 to 150 °C.

CYCLE DETAILS
The cycles of interest included simple cycles with a single heat source and more complicated cycles with two heat sources.

Simple Cycle
The Simple Cycle involves exhaust heat at 520°C being used to heat the coolant water from 85 to 95°C which in turn heats the working fluid to 85°C (Figure 3). This has all the heat entering the cycle at the temperature of the resultant coolant water, 95°C. This cycle is designed to ensure a maximum use of the heat, albeit at a low temperature, and requires a high working fluid mass flow rate. Due to the small temperature difference between the condenser, 50°C, and the boiler, 85°C, the cycle has an inherently low Carnot efficiency of 9.8%. The two key heat exchangers are:
- a high pressure heat exchanger for heating the working fluid with coolant water, and
- a low pressure heat exchanger for heating the coolant water with the exhaust.

This combination of heat exchangers should be relatively low cost because it does not combine the need for high pressure with special materials for the corrosive exhaust. This Simple Cycle features:
- A saturated vapour without any superheat
- A low pressure ratio, ~2.0
- A high mass flow rate.

The Simple Cycle produces a saturated working fluid that boils at a temperature of 5° below the exhaust heated coolant temperature. The solver subroutine adjusts the following parameters to maximise the expander power output:
- Boiling temperature
- Condenser temperature.

A comparison of the model and HYSYS results are given in Table 1.

Superheated Simple Cycle
The Superheated Simple Cycle involves coolant water being used to preheat and boil the working fluid, which is then superheated using the exhaust (Figure 4). To ensure full utilisation of the available heat, the low temperature coolant heat needs to be used to boil the working fluid. Ultimately the maximum temperature will be limited by the temperature at which the working fluid is stable, and this was specified as being 250°C for the hydrocarbon fluids. This Superheated Simple Cycle features:
- The expander inlet pressure being determined by the engine coolant water temperature
- A low pressure ratio ~2 or 3.

The Superheated Simple Cycle introduces the possibility of the working fluid being superheated as it is entering the expander. The solution will depend upon whether the fluid is classified as “wet” or “dry”. For example, alkanes are normally “dry”, because they superheat during expansion and their maximum power output will be without superheat. By contrast, alcohols are normally “wet”, because they condense during expansion and their maximum power output will be with
superheat. The boiler temperature is constrained by the coolant as in the cycle 1, and amount of superheat is limited by the fluid equation of state and thermal stability limits. The solver subroutine adjusts the following parameters to maximise the expander power output:

- Superheat, in this case the boiler temperature is fixed at 85º due to the requirement that the coolant be fully utilised. The expander inlet temperature is the sum of boiling temperature and superheat temperature
- Condenser temperature
- Exhaust, in this subroutine the exhaust is able to be split with some going to boiling more liquid and increasing mass flow, or being used to superheat the vapour. This variable is the amount of heat being directed to the superheating process.

Figure 4. Superheated Simple Cycle – coolant used to preheat and boil with exhaust used to superheat the working fluid

The Superheated Simple Cycle components include (a) an engine, producing coolant and exhaust waste heat streams, (b) a heat exchanger for the coolant to pre-heat and boil the working fluid, (c) a heat exchanger for the exhaust to superheat the working fluid, (d) an expander, (e) a condenser and (f) a pump.

High Temperature Saturated Simple Cycle

The High Temperature Saturated Simple Cycle involves coolant water being used to preheat the working fluid, which is then boiled using the exhaust (Figure 5). Boiling at a high temperature produces a high pressure cycle.

This cycle features a moderate expander inlet temperature, for which the maximum is determined by one of the following:

- Critical temperature of the working fluid
- Minimum approach temperature of the exhaust and working fluid in the heat exchanger
- Any pressure ratio limit for the expander.

The cycle will have a high pressure ratio, ~20, depending on the maximum stable temperature of the fluid.

This cycle has a high Carnot efficiency. For example, if the maximum temperature is 150°C and the condenser temperature is 50°C, the Carnot efficiency is 23.6%. However, since this cycle uses very little coolant heat, the amount of available heat used is small and the available heat conversion efficiency is low.

Figure 5. High Temperature Saturated Simple Cycle – coolant used to pre-heat with exhaust used to boil and superheat the working fluid

The High Temperature Saturated Simple Cycle components include (a) an engine, producing coolant and exhaust waste heat streams, (b) a heat exchanger for the coolant to pre-heat the working fluid, (c) a heat exchanger for the exhaust to boil and superheat the working fluid, (d) an expander, (e) a condenser and (f) a pump.

The High Temperature Saturated Cycle maximises the power output by changing the boiling temperature of the fluid. By adjusting the boiling temperature, the energy of the coolant is not fully utilised. However a large pressure drop across the expander is possible and hence higher power output per mass of working fluid. The solver subroutine adjusts the following parameters to maximise the expander power output:

- Superheat, in this case the boiler temperature is fixed at 85º due to the requirement that the coolant be fully utilised. The expander inlet temperature is the sum of boiling temperature and superheat
- Condenser temperature
- Boiler temperature.

A comparison of the model and HYSYS results are given in Table 2.

Table 2 Comparison of the model results with HYSYS for the High Temperature Saturated Simple Cycle

<table>
<thead>
<tr>
<th></th>
<th>Model</th>
<th>HYSYS</th>
<th>Diff</th>
<th>%Diff</th>
</tr>
</thead>
<tbody>
<tr>
<td>Expander Inlet Pressure kPa</td>
<td>1082</td>
<td>1091</td>
<td>-9</td>
<td>-0.8</td>
</tr>
<tr>
<td>Expander Outlet Pressure kPa</td>
<td>54</td>
<td>53</td>
<td>1</td>
<td>1.9</td>
</tr>
<tr>
<td>Expander Inlet Temperature ºC</td>
<td>171</td>
<td>171</td>
<td>0</td>
<td>0.0</td>
</tr>
<tr>
<td>Expander Outlet Temperature ºC</td>
<td>119</td>
<td>120</td>
<td>-1</td>
<td>-0.8</td>
</tr>
<tr>
<td>Expander Shaft Power Output kW</td>
<td>2.76</td>
<td>2.67</td>
<td>0.09</td>
<td>3.4</td>
</tr>
<tr>
<td>Liquid Flow Rate L/min</td>
<td>3.5</td>
<td>3.2</td>
<td>0.3</td>
<td>9.4</td>
</tr>
</tbody>
</table>
High Temperature Recuperated Cycle

The High Temperature Recuperated Cycle uses coolant to preheat the working fluid, with low temperature exhaust and recuperator used for boiling, and then high temperature exhaust for superheating the working fluid (Figure 6). A recuperator enables high temperature energy recycling within the cycle by capturing some of the heat remaining in the working fluid after it has expanded. While the cycle design may be limited by the thermal stability of the working fluid, use of the recuperator may double the amount of heat that is being absorbed into the cycle as well as reducing the amount of heat rejected through the condenser, leading to a significant improvement in cycle efficiency.

High Temperature Recuperated Cycle features:
- A high expander inlet temperature
- A low pressure ratio, ~2 or 3
- A high internal heat recycle.

This cycle uses the coolant, exhaust heat and a recuperator to increase the enthalpy of the working fluid. The solver subroutine adjusts the following parameters to maximise the expander power output:
- Boiler temperature
- Superheat so the expander inlet temperature is the sum of boiling and superheat temperatures.

Simple Recuperated Cycle

The Simple Recuperated Cycle uses just the gas engine exhaust in conjunction with a recuperator to heat the working fluid (Figure 7). This is similar to the High Temperature Recuperated Cycle without the low temperature heat exchangers. The recuperator partially evaporates the incoming fluid, with the final boiling arising from direct heat exchange with the exhaust.

![Figure 7. Simple Recuperated Cycle – exhaust used in conjunction with a recuperator to heat the working fluid](image)

The Simple Recuperated Cycle components include (a) an engine, using only the exhaust heat stream, (b) a recuperator to pre-heat and boil the working fluid, (c) a heat exchanger for the exhaust to boil and superheat the working fluid, (d) an expander, (e) a condenser and (f) a pump.

This Simple Recuperated Cycle uses only the exhaust heat and a recuperator to increase the enthalpy of the working fluid. The solver subroutine adjusts the following parameters to maximise the expander power output:
- Superheat temperature such that the expander inlet temperature is the sum of boiling and superheat temperature
- Condenser temperature
- Boiler temperature
- Maximum isothermal temperature.
- Mass flow rate.

A comparison of the model and HYSYS results are given in Table 3.

| Table 3 Comparison of the model results with HYSYS for the Simple Recuperated Cycle |
|------------------------------------------|---------|-------|------|------|
| Model | HYSYS | Diff | %Diff |
| Expander Inlet Pressure | kPa | 1082 | 1080 | 2 | 0.2 |
| Expander Outlet Pressure | kPa | 54 | 53 | 1 | 1.9 |
| Expander Inlet Temperature | °C | 171 | 171 | 0 | 0.0 |
| Expander Outlet Temperature | °C | 119 | 119 | 0 | 0.0 |
| Expander Shaft Power Output | kW | 2.76 | 2.79 | -0.03 | -1.1 |
| Liquid Flow Rate | L/min | 3.5 | 3.3 | 0.2 | 6.1 |
VERIFICATION OF MODEL RESULTS

Selected key outputs and results of the spreadsheet models used in this work were compared to the equivalent results from the commercial process engineering software package HYSYS (an ASPEN product). This was performed for each of the five cycles using hexane as the working fluid. The parameters compared were the expander inlet and outlet conditions, the expander shaft power and the flow rate of the liquid working fluid. The value of each of these parameters differed by less than 6% of the HYSYS value, except in one case where it was 9.4%, see selected results in Tables 1 to 3. The parameter with the largest difference varied from cycle to cycle but was either the shaft power output or the liquid flow rate of the working fluid.

It was felt that the spreadsheet model results used in this work may be more reliable than HYSYS results because the thermodynamic data in the NIST REFPROP database is based on real data rather than equations of state.

COMPARISON OF CYCLE RESULTS FOR HEXANE

A comparison of the spreadsheet model results for the different cycles for hexane is given in Table 4. The maximum shaft power output was for the High Temperature Recuperated Cycle, with a value of 3.39 kW. This corresponded to an overall system heat to shaft power conversion efficiency of 8.0%. Since all the available heat was being used in the cycle, the cycle efficiency was also 8.0%.

The High Temperature Saturated Simple Cycle and Simple Recuperated Cycle both had a shaft power output of 2.76 kW. These results are similar because both cycles are constrained by the pressure ratio being <20. The High Temperature Saturated Simple Cycle uses coolant to preheat the fluid, whereas the Simple Recuperated Cycle uses a recuperator. For hexane, both systems create a similar saturated vapour, but other fluids do not.

The Simple and Superheated Simple Cycles do differ in the way in which the exhaust heat is used. The Simple and Superheated Simple Cycles have the same results because, being a dry fluid, no superheat was required to prevent condensation.

CONCLUSION

To utilise waste heat from the dual heat sources of a spark ignition engine in a Rankine Cycle has required detailed consideration of the cycle thermodynamics. This highlighted the challenges to capturing all the heat and producing a high efficiency system due to the low temperature of the coolant and the non-isothermal nature of the exhaust. A number of cycle configurations were proposed which required maximisation of the shaft power output by optimising the total heat utilisation.

Systematic analysis of the candidate cycle configurations and working fluids was needed in order to evaluate the possibilities. A spreadsheet model for each of the candidate cycle was developed by combining the proven thermodynamic data from the NIST REFPROP database with the in-built Solver routine. The results compared well to equivalent results from a commercial process engineering software package. It was felt that the spreadsheet models may be more may be more reliable because the thermodynamic data are based on real data rather than equations of state.

For hexane, the best configuration was the High Temperature Recuperated Cycle which requires several high temperature and high pressure heat exchangers. By comparison the Simple Cycle had the least number heat exchangers and didn’t combine the need for high temperature and pressure in the single unit, but at two-thirds of the power output.

Table 4. Summary of cycle results for hexane

<table>
<thead>
<tr>
<th>Cycle</th>
<th>Expander Inlet Pressure (kPa)</th>
<th>Expander Outlet Pressure (kPa)</th>
<th>Expander Outlet Temperature (°C)</th>
<th>Expander Inlet Temperature (°C)</th>
<th>Pressure Ratio</th>
<th>Pressure Difference (kPa)</th>
<th>Liquid Flow rate (L/m)</th>
<th>Shaft Power Output (kW)</th>
<th>Cycle Efficiency (%)</th>
<th>Available heat conversion efficiency (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple</td>
<td>142</td>
<td>1028</td>
<td>85</td>
<td>54</td>
<td>2.6</td>
<td>88</td>
<td>9.8</td>
<td>2.25</td>
<td>5.3</td>
<td>5.3</td>
</tr>
<tr>
<td>Superheated Simple</td>
<td>1082</td>
<td>119</td>
<td>71</td>
<td>85</td>
<td>2.6</td>
<td>89</td>
<td>9.8</td>
<td>3.5</td>
<td>5.3</td>
<td>5.3</td>
</tr>
<tr>
<td>HT Saturated Simple</td>
<td>2.76</td>
<td>171</td>
<td>71</td>
<td>142</td>
<td>2.6</td>
<td>1028</td>
<td>9.8</td>
<td>2.76</td>
<td>5.3</td>
<td>6.5</td>
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<td>71</td>
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<td>89</td>
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<td>Recuperated Simple</td>
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<td>20</td>
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<td>3.5</td>
<td>13.5</td>
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REFERENCES