



**Under the hood of pocketORC:**  
A guide to modelling organic Rankine cycle (ORC) power systems

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## 1 Overview

pocketORC is a steady-state simulation tool for ORC systems that is based on Python scripts that have been developed for predicting the thermodynamic properties of organic fluids and for simulating ORC power systems. The inputs required to run the pocketORC tool, alongside the outputs generated via the tool, are integrated within a graphical-user interface written in HTML. To call the Python scripts directly from HTML, the open-source PyScript framework is employed. This enables the Python scripts to be uploaded onto the web server and to be run directly from the browser. As such, no installation of any local files is necessary.

An overview of the capabilities of pocketORC is provided in Figure 1. For several fixed inputs that define the heat source and heat sink, alongside component parameters, the user can vary the working fluid and six cycle variables to vary the performance of the system. The model outputs include the power output, mass-flow rate, first- and second-law efficiencies alongside the heat exchanger pinch points and  $UA$  requirements. These are reported in tabular form, alongside a temperature-entropy diagram of the resulting cycle. The tool can simulate different cycle variants, including simple subcritical cycles, recuperated cycles, transcritical cycles and cycles with two-phase expansion. Currently, the working fluids available are R1233zd(E), *n*-pentane and hexamethyldisiloxane (MM).

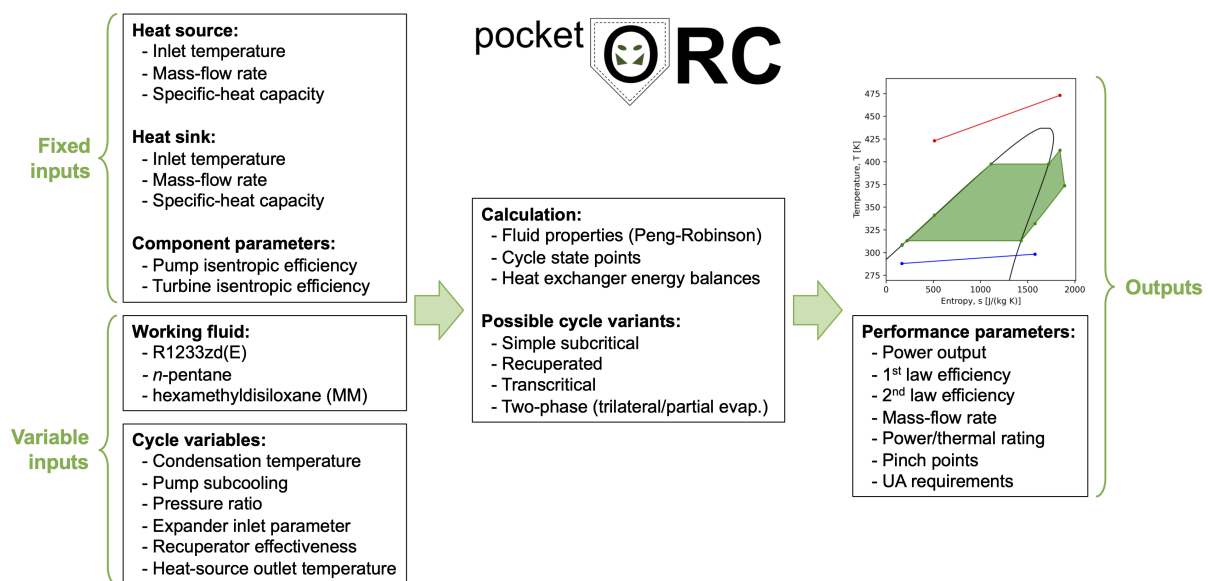


Figure 1: Overview of the modelling capabilities of pocketORC.

Under the hood of pocketORC, there are two Python modules: `thermo_props` and `orc_simulator`. The `thermo_props` module is used to calculate the thermodynamic properties of the working fluid and is based on the Peng-Robinson equation of state. Further details of these calculations are provided in Section 2. The `orc_simulator` module is responsible for simulating the thermodynamic cycle. The starting point is the calculation of the cycle state points. This is described in Section 3 for a simple non-recuperated cycle, whilst extension to recuperated cycles, cycles with two-phase expansion and transcritical cycles is discussed in Sections 4–6. Once the state points are known, the analysis is extended to include the heat source and heat sink, as discussed in Sections 7 and 8, which enables the overall performance of the ORC system to be evaluated. Following this, a more detailed heat exchanger assessment can be carried out to ensure feasible system designs whilst providing an indication of the size of heat exchangers, as discussed in Section 9.

## 2 Thermodynamic properties

### 2.1 Peng-Robinson equation of state

The Peng-Robinson equation of state is one of many cubic equations of state which can be used to model the thermodynamic properties of a working fluid. The equation of state is defined as:

$$p = \frac{RT}{V_m - b} - \frac{a\alpha(T)}{V_m^2 + 2bV_m - b^2}, \quad (1)$$

where  $p$  is the pressure in Pa,  $R$  is the universal gas constant with units J/(mol K),  $T$  is the temperature in K, and  $V_m$  is the molar volume with units of m<sup>3</sup>/mol. The parameters  $a$  and  $b$  are fluid-specific parameters given by:

$$a = \frac{0.45724R^2T_{cr}^2}{p_{cr}}; \quad (2)$$

$$b = \frac{0.0778RT_{cr}}{p_{cr}}, \quad (3)$$

where  $T_{cr}$  and  $p_{cr}$  are the temperature and pressure at the critical point. These terms are derived by setting the derivatives of Eq. 1,  $\partial p/\partial V_m$  and  $\partial^2 p/\partial V_m^2$ , equal to zero at the critical point. The function  $\alpha(T)$  introduces a temperature dependence to the term on the right-hand side of Eq. 1:

$$\alpha(T) = \left(1 + n \left(1 - \sqrt{\frac{T}{T_{cr}}}\right)\right)^2, \quad (4)$$

where  $n$  is a quadratic function of the acentric factor  $\omega$ :

$$n = 0.37464 + 1.54225\omega - 0.26992\omega^2. \quad (5)$$

The acentric factor is another fluid-specific parameter, defined as  $\omega = -\log_{10}(p_r^{\text{sat}}) - 1$ , where  $p_r^{\text{sat}}$  is the reduced saturation pressure at a reduced temperature of 0.7<sup>1</sup>.

Thus, in summary, the relationship between  $p$ ,  $T$  and  $V_m$  for a particular fluid can be predicted based on three parameters which define the fluid, namely the critical temperature  $T_{cr}$ , critical pressure  $p_{cr}$  and acentric factor  $\omega$ .

### 2.2 Internal energy, enthalpy and entropy

The Peng-Robinson equation of state provides the relationship between temperature, pressure and molar volume. However, further information (and calculation) is required in order to compute other thermodynamic properties which are important for thermodynamic analysis, predominantly the internal energy  $e$ , enthalpy  $h$ , and entropy  $s$ .

Thermodynamic properties such as internal energy, enthalpy and entropy do not really have any physical meaning when taken as a single, isolated value. Instead when we talk about these parameters we are actually interested in the difference in internal energy, enthalpy or entropy between two defined points. For this reason these thermodynamic properties are generally calculated relative to an arbitrarily defined reference point. Thus, for a given thermodynamic point, defined in terms of a known temperature, pressure and density, we want to calculate the difference in internal energy,

<sup>1</sup>A reduced parameter is a parameter normalised by the value at the critical point, i.e.,  $T/T_{cr}$  or  $p/p_{cr}$ . For example, at a reduced temperature of  $T/T_{cr} = 0.7$ , the temperature is 70% of the critical temperature.

enthalpy and entropy between this point and the defined reference point. We can calculate this by breaking up the transition from the reference point to the point of interest into three distinct thermodynamic processes. Firstly, the fluid is assumed to expand from the reference point to an infinite volume (i.e., zero pressure) under constant temperature. Following this, the fluid is heated up from the reference temperature to the desired temperature under constant volume. Subsequently, because the fluid remains at zero pressure during this heat addition process it behaves as an ideal gas. Finally, the fluid assumed to be compressed from an infinite volume to the desired volume (i.e., inverse of density) under constant temperature.

Considering these three processes, we can write the change in internal energy as follows, where the first, second and third terms represent the three thermodynamic processes in turn:

$$\begin{aligned}
 e - e_{\text{ref}} = & \int_{V_{\text{m,ref}}}^{\infty} \left( T \left( \frac{dp}{dT} \right)_{V_{\text{m}}} - p \right) dV_{\text{m}} \Big|_{T=T_{\text{ref}}} \\
 & + \int_{T_{\text{ref}}}^T c_{v,0} dT \\
 & - \int_{V_{\text{m}}}^{\infty} \left( T \left( \frac{dp}{dT} \right)_{V_{\text{m}}} - p \right) dV_{\text{m}} \Big|_{T=T}
 \end{aligned} \quad (6)$$

and the change in entropy can be calculated in a similar fashion:

$$\begin{aligned}
 s - s_{\text{ref}} = & \int_{V_{\text{m,ref}}}^{\infty} \left( \frac{dp}{dT} \right)_{V_{\text{m}}} dV_{\text{m}} \Big|_{T=T_{\text{ref}}} \\
 & + \int_{T_{\text{ref}}}^T \frac{c_{v,0} + R}{T} dT - R \ln \left( \frac{p}{p_{\text{ref}}} \right) \\
 & - \int_{V_{\text{m}}}^{\infty} \left( \frac{dp}{dT} \right)_{V_{\text{m}}} dV_{\text{m}} \Big|_{T=T}
 \end{aligned} \quad (7)$$

where the subscript 'ref' refers to the reference point,  $c_{v,0}$  is the ideal specific heat capacity at constant volume, and the derivative  $dp/dT$  can be obtained from differentiating Eq. 1 with respect to temperature.

The change in enthalpy follows from the thermodynamic relationship between  $e$  and  $h$ :

$$h - h_{\text{ref}} = (e - e_{\text{ref}}) + pV_{\text{m}} - p_{\text{ref}}V_{\text{m,ref}} \quad (8)$$

The temperature dependence of the ideal specific-heat capacity at constant pressure  $c_{p,0}$ , and thus the ideal specific-heat capacity at constant volume  $c_{v,0} = c_{p,0} - R$ , is represented using a second-order polynomial:

$$c_{p,0}(T) = A + BT + CT^2. \quad (9)$$

where  $A$ ,  $B$  and  $C$  are constants for a defined fluid. Thus, for a desired fluid, the constants  $A$ ,  $B$  and  $C$  must be specified alongside the critical temperature  $T_{\text{cr}}$ , critical pressure  $p_{\text{cr}}$  and acentric factor  $\omega$ . The definition of these six fluid parameters enables all the thermodynamic properties of the working fluid to be calculated under any thermodynamic condition.

### 2.3 Saturation properties

For our cycle analysis, we also need to be able to determine saturation properties. In particular, for a given saturation temperature (or pressure) we need to be able to calculate the corresponding

saturation pressure (or temperature) and the molar volume, enthalpy and entropy of the saturated liquid and vapour phases. To calculate these properties we introduce the fugacity, which is defined as:

$$\ln \phi = z - 1 - \ln(z - Y) - \frac{X}{2\sqrt{2}Y} \ln \left( \frac{z + (1 + \sqrt{2})Y}{z + (1 - \sqrt{2})Y} \right) \quad (10)$$

where:

$$X = \frac{a\alpha(T)p}{(RT)^2} \quad (11)$$

$$Y = \frac{bp}{RT} \quad (12)$$

and  $z$  is the compressibility factor:

$$z = \frac{pV_m}{RT} \quad (13)$$

Under saturation conditions, the vapour and liquid fugacity are equal and thus, for a known saturation temperature, the pressure that meets this condition needs to be found (or vice versa in the case of a known pressure). This can be found by making an initial assumption for the pressure, from which the corresponding liquid and vapour molar volumes can be obtained by finding the roots of Eq. 1. The corresponding compressibility factors and fugacities can then be obtained for each phase and the pressure updated accordingly using a suitable iterative method. Once the pressure has converged, and the corresponding liquid and vapour molar volumes are known, the internal energy, entropy and enthalpy of the saturated liquid and saturated vapour phases follow from Eqs. 6–8.

## 2.4 A note on units

It is worth noting that the calculations up until have been completed on a molar basis, and therefore the units of internal energy and enthalpy are J/mol and the units of entropy of are J/(mol K). It is possible to conduct all of the calculations within pocketORC on a molar basis. However, within the field of engineering thermodynamics and modelling thermal energy systems it is generally preferred to complete calculations on a kilogram basis. Therefore, the molecular weight of the fluid,  $w_m$  with units of kg/mol, is introduced as a seventh fluid parameter which allows the simple conversion from J/mol and J/(mol K) to J/kg and J/(kg K). The fluid density,  $\rho$  with units kg/m<sup>3</sup>, also follows from the molar volume.

## 2.5 Single-phase flash calculations

The system of equations described so far relates the six thermodynamic properties, namely temperature  $T$ , pressure  $p$ , density  $\rho$ , enthalpy  $h$ , entropy  $s$  and internal energy  $e$  together. Together, they form a set of four equations (i.e., Eqs. 1, 6–8), and thus if we know any two of the six properties we are left with a system of equations that can be solved to obtain the remaining four unknowns.

Any pair of the six thermodynamic variables can be selected, but the pair of properties available influences the complexity of the solution. For example, if the temperature and density (or molar volume) of the fluid are known, then the pressure can be calculated directly from Eq. 1, and the internal energy, entropy and enthalpy follow from Eqs. 6–8. For other pairs, the complexity increases. If, for example, pressure and temperature are known then Eq. 1 becomes a cubic equation involving  $V_m$ , which needs to be solved for the three routes and the appropriate one identified. However, once  $V_m$  is known the calculation of  $e$ ,  $s$  and  $h$  is relatively simple. Things get more complicated when one of either  $e$ ,  $h$  and  $s$  are known alongside  $T$ ,  $p$  or  $\rho$  since iteration becomes necessary in order to solve

the system of equations. The precise details of the numerical methods adopted within pocketORC to solve the equation of state for a given pair of inputs are not detailed here. This is because, for the purpose of understanding pocketORC and the thermodynamics of ORC power cycles, it considered sufficient to just understand the underlying relationships between  $T$ ,  $p$ ,  $\rho$ ,  $h$ ,  $s$  and  $e$ .

To this end, the equation of state module (i.e. `thermo_props`) within pocketORC, can be thought of as black box which for a given pair of inputs,  $x_1$  and  $x_2$ , retrieves the remaining thermodynamic variables:

$$[y_1, y_2, y_3, y_4] = f(x_1, x_2) \quad (14)$$

As we will see in a later section, the main single-phase pairings that we encounter when simulating a thermodynamic power cycle are temperature and pressure, pressure and enthalpy, and pressure and entropy.

## 2.6 Saturation property calculations

When calling saturation properties, the first input is either the temperature or pressure, whilst the second is the desired vapour quality,  $q$ , which is either zero for saturated liquid or unity for saturated vapour. Thus, the calculation returns five outputs which includes the corresponding pressure or temperature, alongside  $\rho$ ,  $e$ ,  $h$  and  $s$ :

$$[p, \rho, e, h, s] = f(T, q) \quad (15)$$

$$[T, \rho, e, h, s] = f(p, q) \quad (16)$$

## 2.7 Fluids currently available in pocketORC

Currently, pocketORC is setup to run with three different working fluids, namely R1233zd(E), *n*-pentane, and the siloxane MM. The corresponding fluid parameters for these three working fluids are summarised in Table 1. These three fluids are included since they are common working fluids considered within the ORC field, and since they have varying critical temperatures one of these fluids is likely to lead to relatively satisfactory performance for most ORC applications.

Table 1: Fluids available in pocketORC.

Fluid	R1233zd(E)	<i>n</i> -pentane	MM	–
$T_{cr}$	439.6	469.7	518.7	K
$p_{cr}$	36.24	33.68	19.31	bar
$\omega$	0.303	0.251	0.418	–
$w_m$	130.5	72.15	162.4	g/mol
$A$	33.35	12.91	64.64	J/(mol K)
$B$	0.282	0.391	0.670	J/(mol K <sup>2</sup> )
$C$	$-0.152 \times 10^{-3}$	$-0.104 \times 10^{-3}$	$-0.290 \times 10^{-3}$	J/(mol K <sup>3</sup> )

### 3 Thermodynamic analysis of a simple ORC system

Throughout this section we will consider the cycle defined in Fig. 1. This figure includes all the notation to describe a subcritical, recuperated ORC system, alongside the heat-source and heat-sink profiles. However, we will start by first introducing a simple non-recuperated cycle, before then moving onto alternative cycles and extending our analysis to the heat source and heat sink.

At this point, we will also make a few key assumptions that help us in our analysis:

- the cycle operates under steady-state conditions, meaning that no component within the cycle accumulates mass and that the steady-state form of energy continuity equation can be used;
- pressure losses within all pipework and heat exchangers are neglected, and thus all heat transfer processes are isobaric, meaning they take place under constant pressure;
- heat losses to the surroundings are neglected, meaning the only heat transfer that takes place is the heat transfer between the working fluid and the heat source and heat sink in the designated heat exchangers.

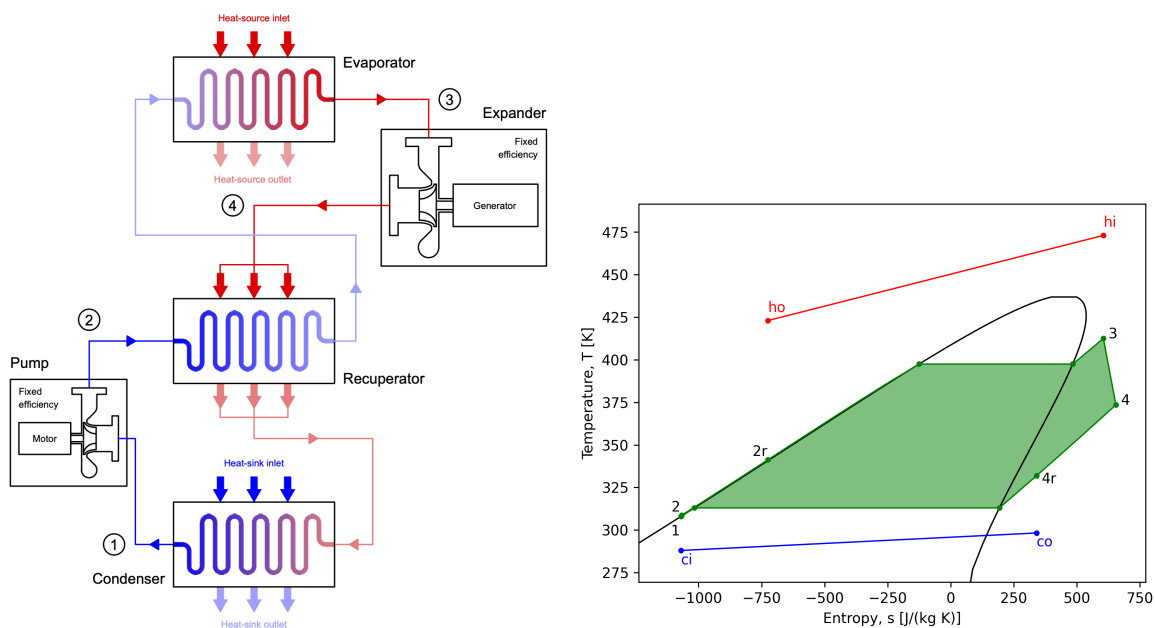


Figure 2: Schematic of a subcritical recuperated ORC system. The left image shows the main components within the cycle and the right figure shows the cycle on a temperature-entropy ( $T - s$ ) diagram. The station numbers 1, 2, 3 and 4 correspond to the pump inlet, pump outlet, expander inlet and expander outlet respectively. The location 'hi', 'ho', 'ci' and 'co' correspond to the heat-source inlet, heat-source outlet, heat-sink inlet and heat-sink outlet respectively.

#### 3.1 Thermodynamic cycle state points

The thermodynamic cycle state points define the thermodynamic properties of the working fluid at the inlet and outlet of each component, and the calculation of these state points forms the principle foundation of the thermodynamic cycle analysis carried out in pocketORC.

A simple cycle, also referred to as a non-recuperated cycle, is constructed from four main components which are the pump, evaporator, expander and condenser. The inlet to each of these components is



denoted by the numbers 1, 2, 3 and 4 respectively.

The thermodynamic properties of the working fluid at these four stations are determined through the specification of four design variables, which effectively define the inlet conditions to the ORC pump and the ORC expander. These variables are:

- the condensation temperature  $T_{\text{cond}}$ , which defines the low pressure of the system;
- the degree of subcooling at the pump inlet  $\Delta T_{\text{sc}}$ , which determines the pump inlet temperature;
- the pressure ratio PR, which defines the change in pressure across the pump and the expander;
- and the amount of superheat at the expander inlet  $\Delta T_{\text{sh}}$ , which defines the expander inlet temperature<sup>2</sup>.

Alongside these four design variables, the isentropic efficiency of the pump  $\eta_p$  and the isentropic efficiency of the expander  $\eta_e$  are also defined as model inputs. The six parameters enable us to calculate all the state points within our cycle.

### 3.1.1 Station 1: Pump inlet

We start with first design variable, the condensation temperature  $T_{\text{cond}}$ , which is the temperature at which we want the working fluid to condense in our cycle and in the process change from gas to liquid. For pure fluids, condensation occurs at a fixed temperature, and every condensation temperature has an associated condensation pressure. Thus, by knowing the condensation temperature we can use our equation of state to retrieve the properties of the working fluid at both the start and end of condensation. For now let's focus on the end of condensation, which is the point at which we have saturated liquid. We will refer to this location using the notation  $1'$ . At this point we know the temperature, and since we have pure liquid we have 100% liquid and the vapour quality is zero. Thus, we can retrieve our other thermodynamic properties at this point:

$$[p_{1'}, h_{1'}, s_{1'}, \rho_{1'}] = f(T_{1'} = T_{\text{cond}}, q_{1'} = 0) \quad (17)$$

Our second variable, the degree of subcooling at the pump inlet  $\Delta T_{\text{sc}}$ , defines the extent to which the working fluid at the pump inlet is colder than the saturation temperature. Thus the pump inlet temperature can be directly calculated from the known condensation temperature and the specified degree of subcooling:

$$T_1 = T_{1'} - \Delta T_{\text{sc}} \quad (18)$$

Moreover, the all our heat exchange processes are isobaric, this means our pump inlet pressure is equal to the condensation pressure. Thus, the properties of the working fluid at the inlet to the pump, station 1, can be readily calculated:

$$[h_1, s_1, \rho_1] = f(T_1, p_1 = p_{1'}) \quad (19)$$

### 3.1.2 Station 2: Pump outlet

The job of the pump is to raise the pressure of the working fluid. The desired pressure increase is defined by our third variable, the pressure ratio PR, and thus the pump outlet pressure is determined from:

$$p_2 = p_1 \times \text{PR} \quad (20)$$

<sup>2</sup>Within pocketORC, the degree of superheat is not defined explicitly as a design variable, but instead the expander inlet parameter is used. This definition of this parameter is described in Section 5.2.

The ideal work associated with this increase in pressure (i.e., the minimum amount of work it takes to achieve this), happens when the pressure increase is reversible and associated with no loss in energy. Such a process is referred to as an isentropic process since entropy is constant for a reversible process. Thus, the conditions following an isentropic, denoted with the subscript 's', can be calculated using the equation of state:

$$[T_{2s}, h_{2s}] = f(p_2, s_1) \quad (21)$$

The pump isentropic efficiency  $\eta_p$ , introduced earlier as a model input, relates the actual specific work of the pump to the ideal specific work, which in turn can be expressed in terms of enthalpy (see Section 3.2):

$$\eta_p = \frac{w_{\text{ideal}}}{w_{\text{actual}}} = \frac{h_{2s} - h_1}{h_2 - h_1} \quad (22)$$

Thus, the actual enthalpy at the pump outlet follows from:

$$h_2 = h_1 + \frac{h_{2s} - h_1}{\eta_p} \quad (23)$$

and the remaining thermodynamic properties once again follow using the equation of state:

$$[T_2, s_2, \rho_2] = f(p_2, h_2) \quad (24)$$

### 3.1.3 Station 3: Expander inlet

Having calculated the pump inlet and outlet conditions, we now turn our attention to the expander for which the analysis follows a similar format to that of the pump. The first step is to determine the evaporation temperature, and the associated conditions where we have saturated vapour in our evaporator (i.e., 100% vapour). We will refer to this location using the notation  $3'$ . Since we assume isobaric heat addition in our evaporator this means the expander inlet pressure equals the pump outlet pressure. Thus, the properties at point  $3'$  are retrieved from the equation of state:

$$[T_{3'}, h_{3'}, s_{3'}, \rho_{3'}] = f(p_3 = p_2, q_{3'} = 1) \quad (25)$$

At this point we can introduce our fourth and final variable, which is the amount of superheat at the expander inlet  $\Delta T_{\text{sh}}$ . This defines the extent to which the working fluid at the expander inlet is hotter than the saturation temperature. Thus, the expander inlet temperature can be calculated from:

$$T_3 = T_{3'} + \Delta T_{\text{sh}} \quad (26)$$

while the remaining thermodynamic state properties at the expander inlet can be readily calculated:

$$[h_3, s_3, \rho_3] = f(T_3, p_3) \quad (27)$$

### 3.1.4 Station 4: Expander outlet

The job of the expander is to reduce the pressure of the working fluid, and extract work in the process. Since we are dealing with a closed cycle, and the rejection process in the condenser is isobaric, this means the expander pressure ratio is equal to the pump pressure ratio, and thus the expander outlet pressure is equal to the pump inlet pressure, i.e.,  $p_4 = p_1$ .

Much like the pump, the ideal work associated with this reduction in pressure, which corresponds to the maximum amount of work that could be generated in such an expansion, happens when the pressure reduction is reversible and associated with no loss in energy. Thus, the ideal expansion

process is an isentropic expansion during which entropy remains constant. Thus, the conditions following an ideal expansion can be obtained from:

$$[T_{4s}, h_{4s}] = f(p_4, s_3) \quad (28)$$

The expander efficiency  $\eta_e$ , which is our second model input alongside our four variables, relates the actual specific work of the expander to the ideal specific work:

$$\eta_e = \frac{w_{\text{actual}}}{w_{\text{ideal}}} = \frac{h_3 - h_4}{h_3 - h_{4s}} \quad (29)$$

and thus:

$$h_4 = h_3 - \eta_e(h_3 - h_{4s}) \quad (30)$$

With the expander outlet pressure and enthalpy known, our remaining thermodynamic properties at the expander can be obtained:

$$[T_4, s_4, \rho_4] = f(p_4, h_4) \quad (31)$$

### 3.2 First law analysis

Having modelled both the pump and expander, we now know the thermodynamic properties of the working fluid at the inlet and outlet of each component within our simple non-recuperated cycle. This allows us to calculate the thermal efficiency of the cycle. The basis for this analysis is the first law of thermodynamics, which we will quickly revise.

The first law of thermodynamics is a form of the conservation of energy law, and arises from the fact that energy cannot be created or destroyed, but instead changes from one form to another. Expressed mathematically for a system under steady-state conditions as follows:

$$Q - W = \Delta U \quad (32)$$

it says that that amount of heat added to a system  $Q$ , minus the work done by the system  $W$  is equal to the change in the internal energy of the system  $\Delta U$ . The internal energy of a system is comprised of thermal energy, or enthalpy, kinetic energy and gravitational- potential energy, and is given as:

$$U = m \left[ h + \frac{c^2}{2} + gz \right] \quad (33)$$

where  $m$  is the mass of the system,  $h$  is the specific enthalpy,  $c$  is the velocity,  $g$  is the acceleration due to gravity and  $z$  is the height. Therefore, considering the scenario in which a system undergoes a change from state A to state B, one can derive the following:

$$Q - W = m \left[ (h_B - h_A) + \left( \frac{c_B^2}{2} - \frac{c_A^2}{2} \right) + g(z_B - z_A) \right] \quad (34)$$

Typically, when we apply the first-law of thermodynamics to any component within a thermodynamic cycle the change in height is negligible, whilst the velocity of the fluid at the inlet or outlet of the component is assumed to be small. Furthermore, the heat addition, work output and mass are given as a rate (i.e. per unit time). Therefore, Equation 2.3 reduces to:

$$\dot{Q} - \dot{W} = \dot{m}(h_B - h_A) \quad (35)$$

where  $\dot{Q}$  is the rate of heat addition with units of J/s,  $\dot{W}$  is the power output with units of J/s, and  $\dot{m}$  is the mass flow rate with units of kg/s.

Often, energy balances may also be defined on a specific basis, where everything is defined on a per unit mass basis. We use lower case to represent this:

$$q - w = h_B - h_A \quad (36)$$

where  $q$  is the specific heat addition and  $w$  is the specific work.

### 3.2.1 Application to the pump and expander

Within the pump of our ORC system, work is added to the system in order to increase the pressure of the working fluid (i.e.,  $p_2 > p_1$ ). This process is also assumed to be adiabatic (i.e., there is no heat loss to the surroundings). Thus, the application of the first law yields:

$$\dot{W}_{\text{pump}} = \dot{m}(h_2 - h_1) \quad (37)$$

Within the turbine of our ORC system, work is extracted from the system, during which there is a reduction in pressure (i.e.,  $p_4 < p_3$ ). Again, this process is assumed to be adiabatic, yielding:

$$-\dot{W}_{\text{expander}} = \dot{m}(h_4 - h_3) \quad (38)$$

which can be rearranged as:

$$\dot{W}_{\text{expander}} = \dot{m}(h_3 - h_4) \quad (39)$$

### 3.2.2 Application to a heat exchanger

Within a heat exchanger of a thermodynamic cycle the working fluid is either cooled or heated and there is no work done, and thus the application of the first law yields:

$$\dot{Q}_{\text{heating}} = \dot{m}(h_3 - h_2) \quad (40)$$

$$\dot{Q}_{\text{cooling}} = \dot{m}(h_4 - h_1) \quad (41)$$

noting the sign change in Eq. 41 due heat leaving the system, rather than being added.

### 3.2.3 Application to the complete cycle

We can of course also apply the first law of thermodynamics to the entire cycle, which encompasses the pressure increase in the pump, the heat addition in the evaporator, the pressure reduction in the expander and the heat rejection in the turbine. Since our ORC is cyclic by definition, the change in internal energy over the entire cycle is zero. Thus:

$$(\dot{Q}_{\text{heating}} - \dot{Q}_{\text{cooling}}) - (\dot{W}_{\text{expander}} - \dot{W}_{\text{pump}}) = 0 \quad (42)$$

which means that the energy entering the cycle must equal the energy leaving:

$$\dot{Q}_{\text{heating}} + \dot{W}_{\text{pump}} = \dot{W}_{\text{expander}} + \dot{Q}_{\text{cooling}} \quad (43)$$

### 3.2.4 Cycle thermal (first law) efficiency

At this point, we can introduce our first useful performance metric, which is the cycle thermal efficiency. This is defined as the amount of work produced by the cycle divided by the amount of

heat that was added. In other words, it is the fraction of the heat that is converted into power. It is thus defined as:

$$\eta_{\text{th}} = \frac{\dot{W}_{\text{net}}}{\dot{Q}_{\text{heating}}} = \frac{\dot{W}_{\text{expander}} - \dot{W}_{\text{pump}}}{\dot{Q}_{\text{heating}}} \quad (44)$$

or expressed in specific form:

$$\eta_{\text{th}} = \frac{w_{\text{net}}}{q_{\text{heating}}} = \frac{w_{\text{expander}} - w_{\text{pump}}}{q_{\text{heating}}} \quad (45)$$

which can be related directly to the calculated values of enthalpy for each of four state points:

$$\eta_{\text{th}} = \frac{(h_3 - h_4) - (h_2 - h_1)}{h_3 - h_2} \quad (46)$$

## 4 Thermodynamic analysis of a recuperated ORC system

The first improvement we can do to our simple, non-recuperated, ORC is to add a recuperator. A recuperator is a heat exchanger that is introduced to recirculate heat within the cycle, which is done by using the hot vapour leaving the expander (station 4) to preheat the cold liquid leaving the pump (station 2). For the same set of thermodynamic variables (i.e.,  $T_{\text{cond}}$ ,  $\Delta T_{\text{sc}}$ , PR and  $\Delta T_{\text{sh}}$ ) the introduction of a recuperator results in the same net work but requires less heat to be added to the cycle leading to an increase in cycle efficiency. As a by-product the amount of heat rejected by the cycle is also reduced which helps to reduce the size of the condenser.

The two inlets into the recuperator correspond to the outlet from the pump (station 2) and the outlet from expander (station 4). We use the notation '2r' and '4r' to denote the two outlets of the recuperator, with station 2r corresponding to the point at which the fluid leaves the recuperator and enters the evaporator and station 4r corresponding to the point at which the fluid leaves the recuperator and enters the condenser. We also note that since our heat exchange processes are assumed to be isobaric, this means that  $p_{2r} = p_2$  and  $p_{4r} = p_4$ .

An energy balance applied to the recuperator yields:

$$\dot{Q}_{\text{recup}} = \dot{m}(h_{2r} - h_2) = \dot{m}(h_4 - h_{4r}) \quad (47)$$

which can be simplified to:

$$h_{2r} - h_2 = h_4 - h_{4r} \quad (48)$$

### 4.1 Recuperator effectiveness

In order to determine the thermodynamic properties of the working fluid at stations 2r and 4r we now introduce our fifth cycle variable, which is the recuperator effectiveness  $\varepsilon$ . The recuperator effectiveness is a useful parameter to define how much heat is transferred between the two fluid streams within the recuperator. It is defined as the ratio of the actual amount of heat transfer that takes place to the maximum amount of heat transfer that is theoretically possible. It can be expressed mathematically as:

$$\varepsilon = \frac{\dot{Q}_{\text{recup}}}{\dot{Q}_{\text{recup,max}}} = \frac{\dot{m}(h_{2r} - h_2)}{\dot{m}\Delta h_{\text{max}}} = \frac{\dot{m}(h_4 - h_{4r})}{\dot{m}\Delta h_{\text{max}}} \quad (49)$$

This can be expressed more simply as:

$$\varepsilon = \frac{h_{2r} - h_2}{\Delta h_{\text{max}}} = \frac{h_4 - h_{4r}}{\Delta h_{\text{max}}} \quad (50)$$

and thus:

$$h_{2r} = h_2 + \varepsilon\Delta h_{\text{max}} \quad (51)$$

$$h_{4r} = h_4 - \varepsilon\Delta h_{\text{max}} \quad (52)$$

Thus, for a defined recuperator effectiveness, which can range between 0 (no heat transfer) and 1 (maximum heat transfer), we can determine the recuperator outlet properties. The only thing that is left is to determine the value for the maximum possible enthalpy change,  $\Delta h_{\text{max}}$ .

#### 4.1.1 Calculating $\Delta h_{\max}$

Formally, the maximum possible enthalpy corresponds to the enthalpy change of the fluid stream with the lower heat-capacity rate when it undergoes the largest possible temperature change, which is defined as the difference between the two inlet temperatures, namely  $T_2$  and  $T_4$ . Thus,  $\Delta h_{\max}$  can be found by computing the corresponding enthalpy change for both streams as they undergo the maximum temperature change and then setting  $\Delta h_{\max}$  to the minimum of the two. For example, for the high pressure fluid leaving the pump we can calculate the enthalpy of the fluid if it was heated up to the expander outlet temperature:

$$h_{2r,\max} = f(p_2, T_{2,\max} = T_4) \quad (53)$$

and similarly for the low pressure leaving the expander we can calculate the enthalpy of the fluid it was cooled down until the pump outlet temperature:

$$h_{4r,\min} = f(p_4, T_{4r,\min} = T_2) \quad (54)$$

Then,  $\Delta h_{\max}$  can be found from:

$$\Delta h_{\max} = \min(h_{2r,\max} - h_2, h_4 - h_{4r,\min}) \quad (55)$$

#### 4.1.2 Understanding $\Delta h_{\max}$

The above set of equations explains the process of finding  $\Delta h_{\max}$ , but they don't necessarily provide the easiest way to understand the underlying physics. So let's consider an example. Let's assume we have a pump outlet temperature of 30 °C and an expander outlet temperature of 50 °C, and for this analysis we will denote these as  $T_{\text{cold}}$  and  $T_{\text{hot}}$  respectively. For sake of simplicity let's also assume that both streams can be treated as fluids that obey the ideal gas law (i.e.,  $h = c_p T$ ) and the specific-heat capacity at constant pressure  $c_p$  of the liquid leaving the pump is 2,000 J/kg K and the  $c_p$  of the vapour leaving the expander is 1,000 J/kg K; let's denote these as  $c_{p,\text{cold}}$  and  $c_{p,\text{hot}}$  respectively.

Now, it should be fairly obvious that if we have a cold stream at 30 °C and a hot stream at 50 °C it is impossible to heat the cold stream to a fluid that is higher than 50 °C. Likewise, it is impossible to cool the hot fluid to a temperature below 30 °C. Thus, the maximum temperature change that can occur is  $50 - 30 = 20$  °C. Now, the maximum enthalpy change of the cold stream is found from:

$$\Delta h_{\text{cold},\max} = c_{p,\text{cold}}(T_{\text{hot}} - T_{\text{cold}}) = 2,000 \times (50 - 30) = 40,000 \text{ J/kg} \quad (56)$$

and similarly for the hot stream:

$$\Delta h_{\text{hot},\max} = c_{p,\text{hot}}(T_{\text{hot}} - T_{\text{cold}}) = 1,000 \times (50 - 30) = 20,000 \text{ J/kg} \quad (57)$$

Thus, if 20,000 J/kg of energy was transferred from the hot fluid to the cold fluid the hot fluid outlet temperature would equal the cold inlet temperature. At this point the condition of thermal equilibrium is met and not more heat transfer is possible since the hot fluid cannot be cooled any further. Thus, it is the minimum of two enthalpy changes that dictates the maximum energy exchange that is possible.

## 4.2 Updated definition for cycle thermal efficiency

For the simple, non-recuperated ORC system we have already introduced the definition for the cycle thermal efficiency. However, this needs to be slightly updated when a recuperator is included. As a reminder, our thermal efficiency, defined in specific form, is:

$$\eta_{\text{th}} = \frac{w_{\text{net}}}{q_{\text{heating}}} = \frac{w_{\text{expander}} - w_{\text{pump}}}{q_{\text{heating}}} \quad (58)$$

Remember that for the same set of thermodynamic variables our state points at the inlet and outlet of the pump and expander are identical in both the simple and recuperated cycles. Therefore, our numerator in the cycle thermal efficiency equation is identical. However, the inclusion of a recuperator reduces the amount of heat added to the cycle in the heater and therefore the denominator is different. More specifically, in a recuperated cycle the heat addition into the cycle starts at station 2r rather than station 2. Thus, our updated cycle thermal efficiency is calculated from:

$$\eta_{\text{th}} = \frac{(h_3 - h_4) - (h_2 - h_1)}{h_3 - h_{2r}} \quad (59)$$



## 5 Thermodynamic analysis of an ORC system with two-phase expansion

Another cycle variation that can be modelled in pocketORC is an ORC operating with two-phase expansion. In this cycle, the expansion process is initiated from a two-phase state (i.e., a mixture of liquid and vapour) rather than from saturated or superheated vapour. This requires a slight modification to the calculation process, and also requires a slight change in our defined cycle variables.

### 5.1 Modelling two-phase expansion

Modelling a cycle with two-phase expansion is based on the same thermodynamic analysis as the simple cycle<sup>3</sup>. The only difference to how the thermodynamic state points at the expander inlet and outlet are calculated.

#### 5.1.1 Expander inlet

Earlier, in Section 3.1.3, we defined the degree of superheat  $\Delta T_{sh}$  and used this to determine the expander inlet conditions. However, this approach is no longer suitable for two-phase expansion since the temperature and pressure are already known. Thus, we now introduce the expander inlet vapour quality,  $q_3$ , as a variable to control the expander inlet condition for two-phase expansion cycles.

Our starting point for modelling two-phase expansion is to determine the saturated liquid and vapour properties at the defined expander inlet pressure. As we have seen previously, we can use our equation of state to retrieve the properties of saturated vapour at a given pressure by setting the vapour quality  $q$  to 1:

$$[T_{3'}, h_{3'}, s_{3'}, \rho_{3'}] = f(p_3, q = 1) \quad (60)$$

Similarly, our saturated liquid properties are retrieved by setting the vapour quality to 0:

$$[T_{2'}, h_{2'}, s_{2'}, \rho_{2'}] = f(p_2, q = 0) \quad (61)$$

Using the thermodynamic definition of vapour quality, the expander inlet conditions are then found the saturated liquid and vapour properties and the defined expander inlet vapour quality:

$$h_3 = h_{2'} + q_3(h_{3'} - h_{2'}) \quad (62)$$

$$s_3 = s_{2'} + q_3(s_{3'} - s_{2'}) \quad (63)$$

$$\frac{1}{\rho_3} = \frac{1}{\rho_{2'}} + q_3 \left( \left( \frac{1}{\rho_{3'}} \right) - \left( \frac{1}{\rho_{2'}} \right) \right) \quad (64)$$

#### 5.1.2 Expander outlet

The expander outlet conditions are found following the same approach described in Section 3.1.4, although the approach needs to be modified slightly in the case that the expander outlet conditions are also two-phase. The first step of the process is to assess whether the conditions after an isentropic expansion are in the two-phase or superheated region. This can be done by determining the properties of saturated vapour at the expander outlet pressure using the equation of state:

$$[T_{4'}, h_{4'}, s_{4'}, \rho_{4'}] = f(p_4, q = 1) \quad (65)$$

<sup>3</sup>Theoretically, a cycle with two-phase expansion could also include a recuperator if the expander outlet condition is in the superheated region. However, the low degree of superheat likely means the potential for internal heat recuperation is limited, and as such recuperated two-phase expansion cycles are not commonly considered.

If the expander inlet entropy is greater than the saturated vapour at the expander outlet pressure (i.e.,  $s_{4'} < s_3$ ), then the expander outlet conditions are in the superheated region and the rest of the calculation process is completed according to Section 3.1.4. However, if  $s_3 < s_{4'}$ , then the conditions after the isentropic expansion are in the two-phase region. As such, the vapour quality after an isentropic expansion is first found from:

$$q_{4s} = \frac{s_3 - s_{1'}}{s_{4'} - s_{1'}} \quad (66)$$

and the corresponding enthalpy is found from:

$$h_{4s} = h_{1'} + q_{4s}(h_{4'} - h_{1'}) \quad (67)$$

Once  $h_{4s}$  the expander outlet enthalpy follows using the specified expander isentropic efficiency, as described in in Section 3.1.4. Once the expander outlet enthalpy is known, a second check is necessary to confirm if the expander outlet condition is still in the two-phase region. This is done by comparing the expander outlet enthalpy to the saturated vapour enthalpy. If  $h_4 > h_{4'}$  then the expander outlet is now in the superheated region and the equation of state can be used directly to determine the expander outlet properties. Otherwise, if  $h_4 < h_{4'}$  then the expander outlet is still in the two-phase region. In this case, the vapour quality at the expander outlet is found from:

$$q_4 = \frac{h_4 - h_{1'}}{h_{4'} - h_{1'}} \quad (68)$$

and thus:

$$T_4 = T_{4'} \quad (69)$$

$$s_4 = s_{1'} + q_4(s_{4'} - s_{1'}) \quad (70)$$

$$\frac{1}{\rho_4} = \frac{1}{\rho_{1'}} + q_4 \left( \left( \frac{1}{\rho_{4'}} \right) - \left( \frac{1}{\rho_{1'}} \right) \right) \quad (71)$$

## 5.2 The expander inlet parameter

So far, we have introduced a simple cycle operating with expansion from a superheated state, and cycle with two phase expansion where expansion starts from a two-phase condition. These two situations are modelled by defining the degree of superheat  $\Delta T_{sh}$ , and the expander inlet vapour quality  $q_3$  respectively. However, looking at the pocketORC calculator you may notice that neither of these two parameters are defined as cycle design variables. This is because having to define two separate variables introduces some challenges when the goal is to have a single model that can model different types of ORC systems.

For this reason, the variable that defines the expander inlet condition is recast in a form which easily allows both types of cycles to be modelled using a single parameter. This parameter is referred to as the expander inlet parameter, and is given the notation  $x_3$ . The expander inlet parameter can take any value between the limits of 0 and 2, and is defined as follows:

- input values between 0 and 1 can be used to model two-phase expansion, and the input value for the expander inlet parameter is linked directly to the expander inlet vapour quality (i.e., expander inlet parameters of 0, 0.5 and 1 would correspond to expander inlet vapour qualities of 0%, 50% and 100% respectively)

- input values between 1 and 2 can be used to model expansion from superheated vapour, and the degree of superheat is defined as a fraction of the maximum possible superheat. The definition takes the form:

$$T_3 = T_{3'} + (x_3 - 1)(T_{hi} - T_{3'}) \quad (72)$$

where  $T_{hi}$  is the heat source inlet temperature, which is introduced in more detail in Section 7. Therefore, if  $x_3 = 1$  then the expander inlet temperature is equal to the evaporation, and if  $x_3 = 2$ , then the expander inlet temperature is equal to the heat source temperature.

## 6 Thermodynamic analysis of a transcritical ORC system

pocketORC is also setup to model transcritical cycles. In a transcritical cycle the analysis is identical to a simple or recuperated cycle except for the fact that the heat addition now occurs at a pressure that is higher than the critical pressure of the working fluid and thus no evaporation (i.e., phase change) occurs.

The only modification to pocketORC that is necessary to enable it to evaluate transcritical cycles is a slight modification to how the expander inlet temperature is determined from on the expander inlet parameter. More specifically, if the pump outlet/expander inlet pressure exceeds the critical pressure, then the expander inlet temperature is defined using the expander inlet parameter and the following definition:

$$T_3 = T_{cr} + (x_3 - 1)(T_{hi} - T_{cr}) \quad (73)$$

where  $T_{cr}$  is the critical temperature of the working fluid.

## 7 Heat-source energy balance

With the exception of the expander inlet parameter, which depends on defining a specific heat-source inlet temperature, our analysis so far has only considered the state points within the cycle. This has enabled the specific work and specific heat addition or rejection of each component to be defined and the cycle thermal efficiency to be calculated. This analysis is helpful to understand how the various cycle variables impact the thermal efficiency of the cycle.

However, for our analysis to be relevant to a practical application we need to extend our analysis to also consider heat source that we have available. The goal then becomes to identify the optimal set of cycle variables that maximises the performance of the overall system.

Within pocketORC, the heat source is defined in terms of an inlet temperature  $T_{hi}$ , a mass-flow rate  $\dot{m}_h$  and a specific-heat capacity  $c_{p,h}$ . For a given application, these three parameters are likely to be known and are therefore fixed inputs. The heat source is assumed to be sensible, in that it is single-phase and any removal of heat corresponds to a reduction in temperature, and the specific-heat capacity is assumed to be constant throughout the heat exchange process. Thus, for a given heat-source outlet temperature  $T_{ho}$ , the amount of heat extracted from the heat source, which is subsequently transferred to the working fluid in the evaporator, follows from the first law of thermodynamics:

$$\dot{Q}_{\text{heating}} = \dot{m}_h c_{p,h} (T_{hi} - T_{ho}) \quad (74)$$

The value selected for the heat-source outlet temperature  $T_{ho}$  will likely depend on the application. For some applications this could be defined as a fixed parameter alongside  $T_{hi}$ ,  $\dot{m}_h$  and  $c_{p,h}$ , whilst in other applications it could be considered a free parameter. In this case, it can be treated as an additional variable alongside the four variables introduced to model a simple ORC system and the recuperator effectiveness. Within pocketORC,  $T_{ho}$  is listed as variable for the sake of generality, but in the case of a pre-defined value this value can simply be entered into the corresponding box and left as a constant.

With the amount of heat transfer known, the mass-flow rate of the circulating working fluid in the ORC system can now be determined through an energy balance applied to the evaporator:

$$\dot{Q}_{\text{heating}} = \dot{m}_h c_{p,h} (T_{hi} - T_{ho}) = \dot{m} (h_3 - h_{2r}) \quad (75)$$

leading to:

$$\dot{m} = \frac{\dot{m}_h c_{p,h} (T_{hi} - T_{ho})}{h_3 - h_{2r}} \quad (76)$$

where a recuperated cycle is assumed. In the case of a simple cycle,  $h_{2r} = h_2$ .

With the mass-flow rate known, the power and thermal rating of all the other components can easily be calculated:

$$\dot{W}_{\text{pump}} = \dot{m} w_{\text{pump}} = \dot{m} (h_2 - h_1) \quad (77)$$

$$\dot{W}_{\text{expander}} = \dot{m} w_{\text{expander}} = \dot{m} (h_3 - h_4) \quad (78)$$

$$\dot{W}_{\text{net}} = \dot{W}_{\text{expander}} - \dot{W}_{\text{pump}} \quad (79)$$

$$\dot{Q}_{\text{recup}} = \dot{m} q_{\text{recup}} = \dot{m} (h_{2r} - h_2) \quad (80)$$

$$\dot{Q}_{\text{cooling}} = \dot{m} q_{\text{cooling}} = \dot{m} (h_{4r} - h_1) \quad (81)$$

## 8 Heat-sink energy balance

The heat sink is modelled in the same way as the heat source, and is defined in terms of an inlet temperature  $T_{ci}$ , mass-flow rate  $\dot{m}_c$  and specific-heat capacity  $c_{p,c}$ . Again, for a given application these conditions are likely to be known. As with the heat source, the heat sink is also assumed to be sensible, in that it is single-phase and any addition of heat corresponds to an increase in temperature, and the specific-heat capacity is assumed to be constant.

For the condenser, an energy balance leads:

$$\dot{Q}_{cooling} = \dot{m}(h_{4r} - h_1) = \dot{m}_c c_{p,c} (T_{co} - T_{ci}) \quad (82)$$

where the only unknown is  $T_{co}$ , which corresponds to the heat-sink outlet temperature. Thus, this can be easily found:

$$T_{co} = T_{ci} + \frac{\dot{m}(h_{4r} - h_1)}{\dot{m}_c c_{p,c}} \quad (83)$$

## 9 Heat exchanger modelling

The analysis described up until covers the thermodynamic analysis of the ORC system that is carried out within pocketORC. The final aspect concerns a slightly more detailed investigation into the heat exchangers. This investigation is necessary to introduce a means to assess and check that the heat exchanger temperature profiles are feasible, in addition to introducing a preliminary means to assess the size of the heat exchangers.

Throughout the analysis completed within pocketORC, it is assumed that all heat exchangers have a counter flow arrangement.

### 9.1 Intermediate heat-source and heat-sink temperatures

For a typical ORC system in which the fluid is subcooled at the inlet to the pump, and superheated at the inlet to the expander, the heat addition and heat rejection processes can be further broken down into three heat transfer processes.

For the heat addition process, the working fluid starts in a subcooled state and is first heated up to the saturation temperature in a process referred to as *preheating*. Following this, the working fluid is evaporated during which it transitions from being in a saturated liquid state to a saturated vapour state, which is a process referred to as *evaporation*. During the final phase, the saturated vapour is heated further until it reaches the desired degree of superheat, which is a process referred to as *superheating*. The properties of the working fluid at each of these points has already been determined. Therefore, we can apply additional energy balances to determine the intermediate temperatures of the heat source:

$$T_{hl} = T_{ho} + \frac{\dot{m}(h_{2l} - h_{2r})}{\dot{m}_h c_{p,h}} \quad (84)$$

$$T_{hv} = T_{ho} + \frac{\dot{m}(h_{3l} - h_{2r})}{\dot{m}_h c_{p,h}} \quad (85)$$

where  $T_{hl}$  and  $T_{hv}$  correspond to the temperature of the heat source at the points where the working fluid is in a saturated liquid and saturated vapour state respectively. Here we have assumed a recuperated cycle, but these equations also apply for a non-recuperated cycle by setting  $h_{2r} = h_2$ .

For the heat rejection process, the working starts in a superheated state at the exit of the expander. During cooling the working fluid is cooled down to a saturated vapour state, converted from saturated vapour to saturated liquid, and the subcooled down to the desired pump inlet temperature. These three processes are referred to as *precooling*, *condensation* and *subcooling* respectively, and again the intermediate heat sink temperatures follow from appropriate energy balances:

$$T_{cl} = T_{ci} + \frac{\dot{m}(h_{1l} - h_1)}{\dot{m}_c c_{p,c}} \quad (86)$$

$$T_{cv} = T_{ci} + \frac{\dot{m}(h_{4l} - h_1)}{\dot{m}_c c_{p,c}} \quad (87)$$

where  $T_{cl}$  and  $T_{cv}$  correspond to the temperature of heat sink at the points where the working fluid is in a saturated liquid and saturated vapour state respectively.

Although perhaps obvious from Eqs. 84–87, it is worth explicitly stating the total heat transferred

for each heat transfer region:

$$\dot{Q}_{\text{preheat}} = \dot{m}(h_{2'} - h_{2r}) = \dot{m}_h c_{p,h}(T_{hl} - T_{ho}) \quad (88)$$

$$\dot{Q}_{\text{evap}} = \dot{m}(h_{3'} - h_{2'}) = \dot{m}_h c_{p,h}(T_{hv} - T_{hl}) \quad (89)$$

$$\dot{Q}_{\text{superheat}} = \dot{m}(h_3 - h_{3'}) = \dot{m}_h c_{p,h}(T_{hi} - T_{hv}) \quad (90)$$

$$\dot{Q}_{\text{precool}} = \dot{m}(h_{4r} - h_{4'}) = \dot{m}_c c_{p,c}(T_{co} - T_{cv}) \quad (91)$$

$$\dot{Q}_{\text{cond}} = \dot{m}(h_{4'} - h_{1'}) = \dot{m}_c c_{p,c}(T_{cv} - T_{cl}) \quad (92)$$

$$\dot{Q}_{\text{subcool}} = \dot{m}(h_{1'} - h_1) = \dot{m}_c c_{p,c}(T_{cl} - T_{ci}) \quad (93)$$

## 9.2 Discretised heat exchanger temperature profiles and pinch points

Having found the intermediate temperatures, we do in theory have enough information to jump to the next section which explains a preliminary method of heat exchanger sizing. However, before doing so, we will go one step further by discretising each of the six heat exchanger processes discussed in the previous subsection, in addition to the recuperator, in order to determine the internal temperature profiles.

### 9.2.1 Pinch point

The first reason we carry out this discretisation process is to determine the point within each heat exchange process at which the temperature difference between the two fluid streams is at a minimum. This point is referred to as the *pinch point*, and identifying this point is important from the point of view of heat exchanger design. The pinch point within any heat exchange process cannot be less than zero; this implies that the temperature of the hot fluid is lower than the cold fluid which is infeasible. Thus, for a given set of ORC variables, if any of the pinch points are below zero, this means that that set of inputs results in an infeasible ORC system. Thus, in the first instance, evaluating the pinch points is an important step to ensuring a feasible ORC system.

In the second instance, the pinch point gives an important indication of the required heat exchanger size. Low pinch points imply very effective heat transfer, but also correspond to larger heat exchanger sizes. On the contrary, high pinch points imply smaller heat exchangers, but also mean that heat transfer is less effective. As a general rule of thumb, it is the goal of the ORC designer to refine the ORC variables in order to maximise the performance of the cycle, whilst bringing the pinch points as close as possible to some minimum value. For example, typical minimum values for pinch points may be set to around 5 or 10 K, but the precise value depends on the application and also the key performance metric of interest.

### 9.2.2 Heat exchanger discretisation

The cycle analysis completed so far only provides the temperatures at the terminals (i.e., the inlet and outlet) of each heat exchanger process. Therefore, considering only the temperature differences at the terminals does not account for the possibility of the pinch point occurring internally within the heat exchanger. To this end, each heat exchange process is further divided, or *discretised*, into a number of smaller heat exchanger elements. Here we will explain the process in the context of the preheater, although the process is essentially the same for all heat exchange process.

In the preheater, the working fluid is heated up from the recuperator outlet temperature  $T_{2r}$  to the saturation temperature  $T_{2'}$ . During this process, the heat-source is cooled down from  $T_{hl}$  to  $T_{ho}$ . Since we assume a counter-flow arrangement, this means the inlet terminal of the working fluid (i.e.,



$T_{2r}$ ) corresponds to the outlet terminal of the heat source (i.e.,  $T_{ho}$ ), and the outlet terminal of the working fluid (i.e.,  $T_{2'}$ ) corresponds to the inlet terminal of the heat source (i.e.,  $T_{hl}$ ).

The first step is to divide the heat exchange process into a number of smaller elements. This is done by equally dividing the total enthalpy change of the working fluid across the desired number of elements:

$$\Delta h = \frac{h_{2'} - h_{2r}}{n} \quad (94)$$

where  $n$  is the desired number of discrete heat exchange elements.

For  $n$  elements, we will end up with a temperature profile defined by  $n + 1$  nodes, and these temperatures can be obtained by applying an energy balance to each discrete element. We will use the notation  $h_{w,i}$ ,  $T_{w,i}$ , and  $T_{h,i}$  to denote the enthalpy of the working fluid and the temperature of the working fluid and heat source at node  $i$  respectively. We will also define our first node as being at the working fluid inlet terminal, and therefore  $h_{w,1} = h_{2r}$ ,  $T_{w,1} = T_{2r}$  and  $T_{h,1} = T_{ho}$ . The enthalpy and temperatures at the next node can then be calculated from:

$$h_{w,i+1} = h_{w,i} + \Delta h \quad (95)$$

$$T_{w,i+1} = f(p_2, h_{w,i+1}) \quad (96)$$

$$T_{h,i+1} = T_{h,i} + \frac{\dot{m}\Delta h}{\dot{m}_h c_{p,h}} \quad (97)$$

The temperature difference at each terminal then follows from:

$$\Delta T_i = T_{h,i} - T_{w,i} \quad (98)$$

from which the minimum value across all the nodes can be easily determined.

As a final note, it is worth noting that pocketORC only returns a single value for the pinch point for the heat addition and heat rejection processes, although each of those processes can be further divided into three different heat transfer regions. In practice, the discretisation process is completed for all three processes, and the value reported in pocketORC is the minimum of the three.

### 9.3 Preliminary heat exchanger sizing

The thermodynamic analysis of the ORC system provides the thermal power exchanged during heat exchange process. For a generic heat exchanger, this can be used to size the heat exchanger through the relation:

$$\dot{Q} = \dot{m}\Delta h = UA\Delta T_{log} \quad (99)$$

where  $\Delta h$  is the change in enthalpy of the working fluid,  $U$  is the overall heat-transfer coefficient,  $A$  is the required heat-transfer area and  $\Delta T_{log}$  is the log-mean temperature difference. The log-mean temperature difference can be calculated using the known temperature profiles and will be discussed in the a following paragraph. This leaves both  $U$  and  $A$  as unknowns. The heat-transfer area is ultimately what we want to determine, but clearly this depends on the value of  $U$ . The overall heat-transfer coefficient is dependent on the flow and thermo-physical properties of the two fluid streams exchanging heat (i.e., velocity, density, viscosity, thermal conductivity etc.) as well as the geometry of the heat exchanger itself. Therefore, using the thermodynamic information derived in pocketORC and without going through a detailed heat exchanger sizing activity, it is difficult to provide precise values for  $U$  and hence determine  $A$ .

For this reason, an alternative approach is to consider the product  $UA$  as a preliminary indicator of heat exchanger size. The assumption here is that when comparing different ORC systems with fairly

similar operating conditions the variation in  $U$  between different designs will be relatively small, and therefore the relative trends in  $UA$  will be representative of the trend in  $A$ . In other words, while  $UA$  does not provide a quantitative indication of the heat exchange size, it does provide a metric against which different ORC systems can be compared.

In order to calculate the  $UA$  value for each heat exchange region (i.e., preheating, evaporation etc.) a discretised model is applied which uses the discretised temperature profiles that have already been determined. Using the same notation introduced in the previous subsection, for a given discrete element  $i$ , the  $UA$  value is obtained from:

$$(UA)_i = \frac{\dot{m}(h_{w,i+1} - h_{w,i})}{\Delta T_{\log,i}} \quad (100)$$

where the log-mean temperature difference is calculated from:

$$\Delta T_{\log,i} = \frac{\Delta T_A - \Delta T_B}{\ln\left(\frac{\Delta T_A}{\Delta T_B}\right)} \quad (101)$$

and:

$$\Delta T_A = T_{h,i+1} - T_{w,i+1} \quad (102)$$

$$\Delta T_B = T_{h,i} - T_{w,i} \quad (103)$$

The total  $UA$  value for a given heat exchange region is then given by summing up all the contributions from each discrete element:

$$UA = \sum_{i=1}^n (UA)_i \quad (104)$$

As with the pinch points, pocketORC returns a single  $UA$  for the heat addition and heat rejection processes. In this instance, the values reported by pocketORC are the summation of the contributions from the different regions:

$$UA_{\text{hot}} = UA_{\text{preheat}} + UA_{\text{evap}} + UA_{\text{superheat}} \quad (105)$$

$$UA_{\text{cold}} = UA_{\text{precool}} + UA_{\text{cond}} + UA_{\text{subcool}} \quad (106)$$

$$UA_{\text{recup}} = UA_{\text{recup}} \quad (107)$$