Working-fluid selection and performance investigation of a two-phase single-reciprocating-piston heat-conversion engine

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Abstract
We employ a validated first-order lumped dynamic model of the Up-THERM heat converter, a two-phase unsteady heat-engine that belongs to a class of innovative devices known as thermofluidic oscillators, which contain fewer moving parts than conventional engines and represent an attractive alternative for remote or off-grid power generation as well as waste-heat conversion applications. We investigate the performance of the Up-THERM with respect to working-fluid selection for its prospective applications. An examination of relevant working-fluid thermodynamic properties reveals that the saturation pressure and vapour-phase density of the fluid play important roles in determining the performance of the Up-THERM – the device delivers a higher power output at high saturation pressures and has higher exergy efficiencies at low vapour-phase densities. Furthermore, working fluids with low critical temperatures, high critical pressures and exhibiting high values of reduced pressures and temperatures result in designs with high power outputs. For a pre-specified Up-THERM design corresponding to a target (CHP prime-mover) application with a heat-source temperature of 360 °C, water is compared with 45 other pure working fluids. When maximizing the power output, R113 is identified as the optimal fluid, followed by i-hexane. Fluids such as siloxanes and heavier hydrocarbons are found to maximize the exergy and thermal efficiencies. The ability of the Up-THERM to convert heat over a range of heat-source temperatures is also investigated, and it is found that the device can deliver in excess of 10 kW when utilizing thermal energy at temperatures above 200 °C. Of all the working fluids considered here, ammonia, R245ca, R32, propene and butane feature prominently as optimal and versatile fluids delivering high power over a wide range of heat-source temperatures.

1. Introduction
Recent trends in global energy use have shown that energy consumption has been increasing, especially amongst developing countries, while, with the exception of the very recent drop in the price of oil, energy prices have been generally rising over the past decades due to a combination of factors, including the growing demand for energy and the gradual reduction in the available reserves of readily accessible fossil fuels [1]. The desire for secure, sustainable, reliable and affordable energy provision in light of increasing energy costs and dwindling resources, along with concerns related to the adverse effects on human health and the environment caused by the release into the atmosphere of gases

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produced from the combustion of fossil fuels, have led to an acceleration of efforts aimed at developing alternative, renewable energy sources, including sources of renewable heat such as solar, geothermal, and (arguably) biomass/biogas [1,2].

In addition, a vast amount of low- to medium-grade (i.e., temperature) ‘wasted’ thermal energy, which is mainly available at significantly lower temperatures than those associated with fossil-fuel combustion (often below \(300 \, ^\circ\text{C}\)), is rejected to the environment in the form of exhaust gases, cooling streams, etc. This energy resource arises from a diverse and broad range of sources in the domestic, commercial, industrial and transport sectors. Recent estimates indicate that over 60% of the overall primary energy supplied globally is rejected in this form; e.g., 59.0 Quads (\(62 \times 10^{18} \, \text{J}\)) of thermal energy was rejected in the US in 2013, which is in excess of the actual national energy consumption (38.4 Quads) by over 50% [3]. Similar figures are reported for Europe and Asia. Therefore, a key component of the energy solution, beyond expanding the utilization of renewable and sustainable energy sources, involves increasing the overall efficiency of fossil-fuel use, thereby reducing both the demand for fossil fuels and the associated emissions. The recovery and re-use of heat has thus been identified as a major pathway towards a high-efficiency and sustainable energy future [1].

Engines capable of utilizing fluid streams at lower temperatures are expected to be inherently inefficient; the Chambadal–Novikov efficiency, \(\eta_{\text{CH-N}} = 1 - \sqrt{T_{\text{sink}}/T_{\text{sat}}} \) [4,5], for heat-source temperatures below 300 °C drops below 30%, and at heat-source temperatures of 100 °C, it is close to 10%. Despite these low efficiencies, the development and utilization of such engines represents an interesting economic proposition since these would provide a means of reducing the rate at which non-renewable energy resources are being depleted, as well as mitigating any environmental (human or natural) impact associated with the use of these resources. For example, we estimate that recovering and re-using waste-heat streams has the potential to provide an additional 8 EJ of energy towards the annual energy consumption in Europe, thereby reducing the annual primary-energy use by over 15%. This would manifest as a direct reduction of the rate at which fossil fuels are being consumed and at which associated emissions are being produced. This example highlights the important opportunities that exist for suitable technologies that can be deployed for heat recovery, re-use and energy integration, e.g., by conversion to useful mechanical, hydraulic or electrical work. In plants that are already in operation the implementation of various waste-heat recovery technologies can lead to important boosts in overall efficiency and utility expenditure savings [6], and in newly built facilities that
incorporate the most up-to-date technologies these savings can potentially be even higher according to theoretical predictions.

In summary, a number of challenges and opportunities continue to act as important drivers behind a strong interest in the utilization of renewable heat and in the recovery and re-utilization of waste heat. The development of high-performance and affordable heat-to-power conversion technologies features prominently as an enabling component of this effort. At the same time, combined heat and power (CHP) is being promoted in various fields of use and scales of application in the interest of improving overall fuel-use efficiency. The main challenge in this case, once again, is the economic viability of a particular project that relies heavily on the upfront (capital) cost of the CHP unit, along with operational performance amongst other factors.

Several thermodynamic cycles have been studied in the context of low-temperature power generation, including the organic Rankine cycle (ORC) [7–14], the Kalina cycle [15–18], the Goswami cycle [19,20], supercritical carbon dioxide cycles (s-CO2) [21,22] and trilateral cycles [23–25]. Over the years, other novel cycle configurations have also been proposed for waste-heat recovery (WHR) applications. These include various thermoacoustic and thermofluidic heat engines [26–29] and phase-change heat engines such as the Non-Inertive-Feedback Thermofluidic Engine (NIFTE) [30–36]. More recently, the Up-THERM engine [37] has been proposed by Encontech [38] and is being developed by a consortium of European researchers and SMEs [39–41]. This engine belongs to a class of unsteady vapour-phase heat engines referred to as ‘two-phase thermofluidic oscillators’ (TFOs). When a steady temperature difference is applied across a TFO, the working fluid within this device experiences sustained thermodynamic-property (i.e., pressure, volume and temperature) oscillations, while undergoing phase change during heat addition and rejection. These sustained oscillations can then be harnessed to drive a generator or a load, where work can be extracted.

Non-steam Rankine cycles differ from steam Rankine cycles chiefly in the choice of the working fluid. ORCs utilize organic fluids (e.g., hydrocarbons and refrigerants) and their mixtures, the Kalina cycle utilizes a mixture of water and ammonia, while the s-CO2 cycle utilizes supercritical carbon dioxide as the working fluid. One of the features of WHR heat engines is the deployment of a broad range of fluids (including hydrocarbons, refrigerants, siloxanes), which allows engineers to select and/or tune certain (combinations of) fluids depending on the characteristics of the heat source, and the heat sink where relevant. The available fluids are classified into three categories based on the slope of the dew-point curve in a temperature–entropy (T–s) plot. Fluids that show a negative-slope dew-point curve on the T–s diagram are classified as wet fluids, e.g., water, while those with a positive-slope dew-point line, e.g., hexane, are dry fluids. The third class are those with a constant entropy, regardless of temperature, along the dew-point line, e.g., benzene and they are regarded as isentropic fluids.

An experimentally validated model of the Up-THERM engine was presented by Kirmse et al. [37] where the key physical characteristics of the engine were studied. Using this model, we present here a characterization of the engine with respect to optimal working fluids. Thus, the novelty and scientific contribution of this work, and where it goes beyond the previous effort by Kirmse et al. [37] are:

- Optimal characterization of the engine load;
- Thermodynamic property characterization of the engine;
- Comparison with other established technologies, including the NIFTE, ORC and Stirling engines;
- Performance improvement on the nominal engine design via working-fluid selection; and
- Optimal working fluid selection for prospective applications.

Specifically, we investigate the effects of key working-fluid properties on the performance indices of the engine and then investigate a series of potentially viable working fluids that can be employed in the engine. Important heat-transfer characteristics (e.g., boiling and condensation heat-transfer coefficients, heat exchanger areas) and thermodynamic performance indices such as the power output and the exergy efficiency are highlighted.

We then conclude by exploring the viability of the engine for power generation at off-design conditions by considering the effect of the variations in heat-source temperature on the optimal working-fluid(s) selection. Ultimately, these will provide guidance on working fluid(s) selection based on the characteristics of the heat source, heat sink and operating conditions (including the application and location) of the Up-THERM heat conversion engine.

2. Up-THERM heat engine
2.1. Device description and operation

The key components of the Up-THERM heat engine are depicted in Fig. 1. It consists of hot and cold heat-exchanger sections, which are part of the vertical displacer cylinder on the left-hand side of the device as it appears in this figure. This is where heat is either added from or rejected to an external source or sink, respectively. The device contains a working fluid in both the liquid and vapour phases; working fluid in the vapour phase is present at the top part of the displacer cylinder as shown in the inset of Fig. 1 where the piston is at the bottom dead centre (BDC), while the rest of the

![Fig. 1. Schematic of the Up-THERM heat engine with hot and cold heat exchangers, piston, valve, mechanical springs and hydraulic motor with piston at the top dead centre (TDC) and at the bottom dead centre (BDC, inset). The top space of the hydraulic accumulators is filled with air.](image-url)
engine is filled with working fluid in the liquid phase. In particular, the quantity of vapour at the top of the displacer cylinder acts as a gas spring, which is periodically compressed and expanded as the vapour–liquid interface (or, liquid level) below it, and the so called ‘liquid piston’ in the displacer cylinder, oscillate vertically, thus contacting the hot and cold heat-exchanger surfaces where evaporative and condensing phase-change heat transfer occurs in an alternating manner. Within the displacer cylinder is also a solid piston; the position of this piston, together with the inner wall of the displacer cylinder, forms the piston-valve arrangement that separates the displacer cylinder into upper and lower chambers. Beneath the piston valve sits a slide bearing. A mechanical spring just below the solid piston connects the bottom of the piston to the bottom of the displacer cylinder, which is also connected to a liquid connection-tube. At the other side of the connection tube the flow is split into two ends of the same closed fluid-loop that forms the load arrangement. This contains two check valves, two hydraulic accumulators, and a hydraulic motor where work is generated.

It is assumed that the cycle starts with the piston at the top dead centre (TDC) position, as in Fig. 1. In this position, the vapour–liquid interface in the displacer cylinder is in contact with the hot heat-exchanger (HHX) surface, which causes the liquid working fluid to be evaporated, thus increasing the pressure in the gas (vapour) spring above it. This, together with the force from the upper section of the mechanical spring that is initially fully compressed, forces the piston and vapour–liquid interface downwards. As this takes place, the piston valve closes, thereby preventing fluid from flowing from the upper to the lower chamber. From this point the pressure in the upper chamber continues to increase, while the piston continues to move downwards with the valve closed. After a certain vertical (downwards) displacement of the piston, the piston valve opens, which suddenly re-connects the two (upper and lower) chambers of the displacer cylinder; the large pressure differential between the chambers causes fluid to flow quickly from the upper into the lower chamber. Due to inertia, the vapour–liquid interface and solid piston overshoot their equilibrium position—which lies between the HHX and cold heat-exchanger (CHX) surfaces, and equivalently, at the mean vertical position of the vapour–liquid interface in the displacer cylinder—bringing the interface and the vapour directly above in contact with the cold surface of the CHX and compressing the lower section of the mechanical spring.

This causes working-fluid vapour to condense thereby decreasing the pressure in the gas (vapour) spring, and therefore in the entire displacer cylinder. The resulting suction force pulls the solid piston and the vapour–liquid interface upwards (with the aid of the force in the compressed lower mechanical spring) and, eventually, closes the piston valve after a certain vertical (upwards) displacement of the piston. The valve remains closed as the piston continues to move upwards, within a certain range. For as long as the valve is closed, and since condensation continues to occur, the pressure in the upper chamber of the displacer cylinder continues to decrease. At some point, the piston valve re-opens and a sudden flow of working fluid from the lower chamber into the upper chamber allows the pressures of the two chambers to be equalized once again. The piston and vapour–liquid interface reach the HHX and the cycle is complete.

The oscillating (zero-mean) fluid flow in the displacer cylinder is transmitted via the connection tube to the load arrangement, where it is transformed into a unidirectional flow with the use of two check valves. The two hydraulic accumulators act to dampen the amplitudes of the pressure and flow oscillations in the load arrangement. Hence, a more steady flow can be supplied to the hydraulic motor, where useful work can be extracted from the device at higher efficiency (thanks to the dampered unsteadiness).

### 2.2. Mathematical model development

The Up-THERM engine model development, presented in detail by Kirmse et al. [37], follows previous approaches for thermoacoustic and thermofluidic devices by Ceperley [26], Huang and Chuang [27], Backhaus and Swift [28,29] and, in particular, Smith and Markides [30,42–44] who developed various models for the NIFTE device [30–35] to which the Up-THERM engine has some similarity. These authors reported that the operating oscillation frequency \( f \), thermal gain (related to the temperature or heat gradient along the walls of the heat exchangers of the device) \( k \), and exergy efficiency \( \eta_{ex} \) predicted by the NIFTE models were in good agreement with experimental data from an early-stage NIFTE prototype that took the form of a thermally powered fluid-pump. Since the thermal energy exchanged between the HHX/CHX walls and the working fluid in both the NIFTE and the Up-THERM engine are dominated by alternating phase-change (evaporation and condensation) heat transfer, the modelling approach used for the NIFTE is a suitable starting point for the Up-THERM engine model development.

Briefly, the dominant thermal or fluid process in each spatially lumped component of the Up-THERM is described to first-order by an ordinary differential equation (ODE). This allows electrical analogies to be drawn such that thermal and fluid resistances can be represented by electrical resistances \( R \), liquid inertia by inductances \( L \), and hydrostatic pressure and vapour compressibility by capacitances \( C \). The models for the vertical motion of the solid piston and the flows in the slide-bearing, liquid-column, connection tube, hydraulic accumulators and the hydraulic motor are linearized based on the assumption of small variations around their time-mean values, which define the operating equilibrium point (detailed in Section 2.2.1). The temperature profile along the heat-exchanger walls is assumed to follow a (non-linear) \( \tanh \) function; this assumption has been validated experimentally in Kirmse et al. [37]. The piston valve and check valves exhibit inherently and strongly non-linear behaviour with large variations around their equilibrium points; they are thus modelled as non-linear components (detailed in Section 2.2.2).

#### 2.2.1. Linear components

The solid piston (and surrounding fluid flow inside the displacer cylinder) are modelled by combining the force balance equation on the piston with the Navier–Stokes equation for the fluid. The Navier–Stokes equation is reduced by assuming fully developed, incompressible and axisymmetric flow. Below the piston valve lubricated by a thin liquid-film while the bulk of the liquid flows with experimental data from an early-stage NIFTE prototype that the Up-THERM engine is dominated by alternating phase-change (evaporation and condensation) heat transfer, the modelling approach used for the NIFTE is a suitable starting point for the Up-THERM engine model development.

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\[
\begin{align*}
R_1 &= \frac{128c_2 l_2 \mu}{\pi c_1 c_3}, \quad R_2 = \frac{128c_2 l_2 \mu}{\pi c_1 (c_1 - 2c_2 d_p^2)}, \quad C_1 = \frac{\pi^2 c_1 (c_1 - c_2 d_p^2)}{64c_2^2 k_m}, \\
L_1 &= \frac{64c_2^2 l_2 m_p}{\pi^2 c_1 (c_1 - 2c_2 d_p^2)}, \quad R_p = \frac{64l_2 \mu}{\pi d_p c_1}, \quad C_p = \frac{\pi^2 d_p^2 c_1}{32k_m c_2}, \quad L_p = \frac{32m_p c_2}{\pi^2 d_p^2 c_1}, \\
R_{bp} &= \frac{16l_2 h_b}{\pi^2 d_p^2 \delta}, \quad L_{bp} = \frac{4l_2 h_b}{\pi d_p^2}, \quad L_{b1} = \frac{4l_2 h_b}{\pi d_p^2}, \quad L_{b2} = \frac{128l_2 h_b}{\pi d_p^2}.
\end{align*}
\]

In Eq. (1), \( c_1 = d_p^2 - d_b^2, \quad c_2 = l_2 \), \( d_p = d_p / d_b \), and \( c_3 = c_3 (d_p^2 + d_b^2) - c_1 \) are geometric constants, \( h_b \) and \( d_p \) are the height/length and diameter of the solid piston, and \( m_p \) and \( \rho_m \) its mass and density, respectively. In addition, the slide bearing has length \( h_b \) and diameter \( d_b \), and the spring constant is \( k_m \).
Liquid columns are modelled by applying the Navier–Stokes equation, simplified with the same assumptions as for the modelling of the liquid surrounding the piston. Based on this approach, the resistance, inductance and capacitance of each liquid column are given by:

\[ R = \frac{128 \mu l_0}{\pi d_0^2} \; ; \quad L = \frac{4 \rho l_0}{\pi d_0^2} \; ; \quad C = \frac{\pi d_0^4}{4 \rho g}, \]  

(2)

where the length of the liquid column is represented by \( l_0 \), its diameter by \( d_0 \), the viscosity and density of the liquid in the column by \( \mu \) and \( \rho \), and \( g \) is the gravitational acceleration. It should be noted that the hydrostatic pressure difference only applies for the liquid column in the displacer cylinder, as the other cylinders are completely filled with liquid and thus have constant liquid-column height.

The hydraulic accumulators are modelled as linear gas springs. It is assumed that the gas at the top of the accumulator is compressed/expanded isentropically and therefore, based on an ideal-gas approximation, the process obeys \( PV^\gamma = \text{const.} \), and the capacitance of each accumulator gas spring is:

\[ C = \frac{V_0}{\sqrt{T_0}} \]  

(3)

where \( V_0 \) and \( T_0 \) respectively are the equilibrium volume and pressure of the gas in the accumulators.

A torque balance is applied on the motor, which leads to the frictional losses and inductance of the motor:

\[ R_{\text{fric}} = \frac{16 \mu_{\text{gen}} \pi d^4 l}{\pi c_d d_{\text{in}}}, \quad L_{\text{fric}} = \frac{8 m_{\text{in}}}{\pi^2 q_d^2}, \]  

(4)

where \( \mu_{\text{gen}} \) is the viscosity of the lubricant around the shaft, \( l \) and \( d \) the length and diameter of the shaft, \( c \) the gap between the motor and the shaft, \( d \), the diameters of the inlet and outlet pipes of the motor, and \( d_{\text{in}} \) and \( m_{\text{in}} \) the diameter and homogeneously distributed mass of the motor. The useful instantaneous mechanical power that can be extracted from the device is dissipated in a further electrical resistance \( R_{\text{gen}} \):

\[ W = R_{\text{gen}} U_{\text{in}}^2, \]  

(5)

where \( U_{\text{in}} \) is the (volumetric) fluid flow-rate through the hydraulic motor, and \( R_{\text{gen}} \) is determined empirically to maximize the power output from the Up-THERM converter, as described in Section 2.4.2. We do not differentiate in this work between mechanical and electrical power output.

Other performance indices useful in characterizing the Up-THERM engine, in particular a few efficiency measures, are defined in Section 2.3. A detailed description of the modelling approach for the hydraulic motor and the other linear components can be found in Kirmse et al. [37].

2.2.2. Non-linear components

In the thermal domain, the temperature profile along the HHX–CHX heat-exchanger surfaces that are in contact with the working fluid is modelled by using a tanh(.) function that saturates when the vapour–liquid interface position \( y \) moves far away from the equilibrium position at \( y = 0 \), as shown in Fig. 2 [34]:

\[ T_{\text{hx}} = \alpha \tanh(\beta y). \]  

(6)

In Eq. (6), \( \alpha \) is half of the maximum temperature difference between the HHX and CHX, and the product \( \beta \) is the gradient of the temperature profile at and close to the origin, as defined in Fig. 2.

The rate of thermal energy exchanged between the heat exchangers and the working fluid can be described via a convective (phase-change) heat transfer coefficient \( h \),

\[ Q = hA_{\text{hx}}(T_{\text{hx}} - T_{\text{sat}}) \approx T_0 \dot{S}, \]  

(7)

with \( T_0 \) the equilibrium temperature, \( \dot{S} \) the corresponding entropy flow-rate, \( A_{\text{hx}} \) the area over which phase-change heat transfer occurs, and \( T_{\text{sat}} \) the working-fluid temperature.

The thermal domain must be coupled to the fluid domain, as the rest of the engine is described in the fluid domain. Two coupling equations are employed for this purpose [30]:

\[ \dot{S} = \rho_v S_q U_{\text{th}}, \]  

(8)

\[ T_{\text{hx}} = \left( \frac{dT}{dP} \right)_{\text{sat}} P_{\text{th}} \; ; \quad T_{\text{sat}} = \left( \frac{dT}{dP} \right)_{\text{sat}} P_{\text{cv}}. \]  

(9)

In the above equations, \( \rho_v \) is the density of the working fluid in the vapour phase, \( S_q \) is the phase-change specific entropy, \( U_{\text{th}} \) is the volumetric flow-rate, \( (dT/dP)_{\text{sat}} \) is the rate of change of temperature with pressure in the saturation region of the working fluid, and \( P_{\text{th}} \) and \( P_{\text{cv}} \) are the pressures in the thermal domain and the gas (vapour) spring at the top of the displacer cylinder, respectively.

Thus, the volumetric flow-rate due to heat exchange (leading to evaporation/condensation) becomes:

\[ U_{\text{th}} = \frac{P_{\text{th}} - P_{\text{cv}}}{R_{\text{th}}}, \quad R_{\text{th}} = \frac{\rho_v S_q T_0}{hA_{\text{hx}}(dT/dP)_{\text{sat}}}, \]  

(10)

where \( R_{\text{th}} \) is the thermal resistance.

The piston valve in the displacer cylinder is modelled by using a combination of two Heaviside step-functions to account for the two instances in the cycle where the valve opens/closes:

\[ R_{\text{pv}} = R_{\text{min}} + \left\{ \frac{1}{2} R_{\text{max}} \left( -H(P_{\text{cv}} - \rho_{\text{sat}} g h) + H(P_{\text{cv}} + \rho_{\text{sat}} g h) \right) \right\}. \]  

(11)

In Eq. (11), \( R_{\text{min}} \) is a constant minimum resistance due to viscous drag when the valve is open and \( R_{\text{max}} \) a large pre-set constant resistance applicable when the valve is closed. In addition, \( P_{\text{cd}} \) is the hydrostatic pressure of the liquid column inside the displacer cylinder, \( \rho_{\text{sat}} \) is the density of the working-fluid liquid and \( h \) is the distance of the solid piston from its time-mean equilibrium position.

The check valves in the load arrangement are also modelled using a Heaviside step-function. Each check valve remains opened when there is a positive fluid flow-rate \( U \) through it and closes at the moment when the flow rate becomes negative:

\[ R_{\text{cv}} = R_{\text{max}} H(U). \]  

(12)
A third non-linear resistance is introduced to ensure that the amplitudes of the piston and liquid flow in the displacer cylinder are not larger than the geometric dimensions (height) of the displacer cylinder:

$$R_{nl} = R_{max} \left( -H(P_{Cd} - \rho_w gh_3) + H(P_{Cd} + \rho_w gh_3) \right),$$

where $h_3$ is the maximum allowable amplitude by this expression.

Finally, the models of all individual components are then interconnected in the same way as they are in the physical engine, resulting in the circuit diagram shown in Fig. 3.

### 2.2.3. Heat transfer coefficient

Eq. (7) describes the heat input from the heat source to the working fluid. This process involves evaporative heat transfer to boil the working fluid, and is taken as a pool-boiling process in this work. Thus, a key parameter to be evaluated for this process is the pool-boiling heat transfer coefficient, $h$. The heat transfer coefficient $h$ can be calculated by using the reference heat transfer coefficient for a specific fluid $h_0$ and a correlation for the reduced heat transfer coefficient [45]:

$$h = \frac{q}{h_0} = F_p F_w.$$

For most fluids experimental values of $h_0$ exist, and are available from Table 1 of Section H2 in the VDI Heat Atlas [45]. For fluids for which experimental values do not exist, a calculation procedure is presented in the VDI Heat Atlas. In Eq. (14) the functions $F_p$ and $F_w$ are dimensionless and independent of the fluid. They take into account the heat flux, the reduced pressure ($p_r = p/p_r$) of the fluid, and the properties of the heat-exchanger wall. The function $F_p$ is dependent on the heat flux $q$, the reference heat flux $q_0 = 20$ kW m$^{-2}$, and an exponent $n$ that is dependent on the reduced pressure and the fluid properties:

$$F_p = \left( \frac{q}{q_0} \right)^n,$$

where $n$ is given by:

$$n = \begin{cases} 0.9 - 0.3p_r^{0.15}, & \text{for water} \\ 0.95 - 0.3p_r^{0.3}, & \text{for organic fluids} \end{cases}$$

The function $F_p$ takes the pressure dependability of the reduced heat-transfer coefficient into account. It is calculated as:

$$F_p = \left( 1.73p_r^{0.27} + 6.1p_r^{0.68}((1 - p_r)) \right)^2 \frac{1}{C_{18}/C_{19}}, \text{ for water}$$

$$F_p = \left( 0.7p_r^{0.2} + 4p_r + 1.4p_r/((1 - p_r)) \right)^2 \frac{1}{C_{18}/C_{19}}, \text{ for organic fluids}.$$

The function $F_w$ takes the properties of the heat-exchanger material into account. It can be split into a function $F_{wm}$, which considers the surface roughness of the heat-exchanger wall, and a function $F_{wr}$ that considers the wall material, so that $F_w = F_{wm}F_{wr}$. $F_{wm}$ can be calculated by:

$$F_{wm} = \left( \frac{b}{b_0} \right)^{0.5},$$

where $b_0 = 0.4$ μm is the reference surface roughness for metal surfaces, $b$ is the measured surface roughness. This value is not known then $R_o = R_{ao} = 0.4$ μm, so that $F_{wm} = 1$ [46]. The function $F_{wm}$ accounts for the wall material by using the ratio of the effusivity $b = \sqrt{\rho c}$ of the wall material to the effusivity of the reference material, copper $b_0 = 35.35$ kW m$^{-2}$ K:

$$F_{wm} = \left( \frac{b}{b_0} \right)^{0.5}.$$

### 2.3. Performance indices and efficiency definitions

Four indicators—oscillating frequency ($f$), power output ($P = W$), exergy efficiency ($\eta_{ex}$) and thermal efficiency ($\eta_{th}$)—are used to describe the performance of the Up-THERM device. Of these, the oscillating frequency is unique to unsteady thermofluidic heat engines such as the NIFTE and the Up-THERM. The power output and efficiencies, on the other hand, are commonly encountered performance indicators used in describing heat engines in

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**Fig. 3.** Circuit diagram of the Up-THERM heat engine; colours correspond to the engine components in Fig. 1. $R$ denotes a resistance, $L$ an inductance and $C$ a capacitance. $U$ is the volumetric flow-rate through a component. The subscript ‘th’ denotes the thermal domain. The single components of the fluid domain are the leakage flow denoted by ‘tl’, the piston ‘p’, the fluid flow in the slide bearing ‘bl’, the piston in the slide bearing ‘bp’, the connection tube ‘c’, the liquid column ‘d’ and the gas spring ‘v’ in the displacer cylinder, and the non-linear valve formed by the piston and cylinder ‘pv’. The load comprizes the two check valves ‘cv’, I, two pipes ‘c’, I, hydraulic accumulators ‘a, i’ and hydraulic motor ‘hm’. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
The physical dimensions of the Up-THERM engine were considered in Kirmse et al. [37], with water as the working fluid. Here, in Table 1, we list the resulting nominal electrical parameters (resistances, capacitances and inductances) from that work. These parameters directly correspond to those in Fig. 3 and most of them remain unchanged in the present work. Those that depend on the heat-source temperature and the thermodynamic properties of the working fluid (highlighted by "**" in Table 1), change accordingly. A numerical simulation of the model (using ODE solvers in MATLAB [34,47,48]) with the nominal parameters in Table 1 results in the nominal performance of the engine presented in Table 2.

The time-varying volumetric flow-rates in key engine sections during nominal operation are shown in Fig. 4a. It can be observed that a limit cycle is attained from about 2.5 s; after initial transients in pressures and flow rates, the oscillations are sustained at a constant frequency and amplitude. In this figure, $U$ is the volumetric (liquid) flow-rate through the displacer cylinder and into the connection tube (which is also equal to the flow rate from the connection tube to the load arrangement) and $U_{piston}$ represents the movement of the piston in the displacer cylinder. Both of these flow rates are seen to oscillate about a mean value of zero, with $U_{piston}$ having larger amplitudes than $U$ due to leakage around the piston and through the slide bearings. Furthermore, $U_{final}$ is the volumetric (liquid) flow-rate through the check valve that 'feeds'
the hydraulic motor. This flow is always positive with the same peak amplitude as $U$ due to the non-return action of the valve that prevents $U_{\text{pist}}$ from having a significant negative amplitude since only a small amount of liquid can flow back before the valve closes. When the valve is fully open, the flow rates $U_{\text{pist}}$ and $U$ are identical. This means that all the liquid from the displacer cylinder and via the connection tube flows through the check valve into the accumulator and the hydraulic motor. Downstream of the accumulator the volumetric (liquid) flow-rate $U_{\text{gen}}$ is equal to the flow rate through the hydraulic motor, and this is always positive due to the action of the check valves providing uni-directional flow. It does, however, experience reduced amplitudes of oscillation due to the dampening action of the two hydraulic accumulators.

Time-varying pressures in important engine sections are shown in Fig. 4b. In particular, $P_{\text{C1,ac}}$ is the hydrostatic pressure of the liquid column in the displacer cylinder below the piston, and is thus a measure of the height of the liquid column below the piston. The amplitude of $P_{\text{C1,ac}}$ is smaller than that of the piston pressure $P_{\text{pist}}$ and that of the pressure in the hydraulic accumulator $P_{\text{acc1}}$. $P_{\text{pist}}$ is the pressure exerted by the compressed mechanical springs and therefore it represents the piston position in the displacer cylinder. The highest pressure amplitude can be observed in the piston as it is directly connected to the displacer cylinder where the phase change and resultant pressure forcing arises.

2.4.2. Optimal load characterization

While the nominal electrical analogy parameters (RLCs) of the Up-THERM engine have been defined, the load resistance $R_{\text{gen}}$ is yet to be determined as it is external to the engine. This is the resistance presented by the employed generator, and the power extracted from the engine is strongly correlated with this parameter. It would be expected that there is a value of $R_{\text{gen}}$ that optimizes some performance criterion of the engine. Thus, the optimal $R_{\text{gen}}$ needs to be defined relative to the performance criterion, e.g., maximum power output or maximum efficiency; here we use the maximum power output. This is especially important in waste-heat recovery applications, where the aim is to maximize power output per unit cost [7].

The power output from the engine is defined in Eqs. (5) and (20). From these relations, one would expect higher power outputs at higher values of $R_{\text{gen}}$, as the power output appears to be directly proportional to $R_{\text{gen}}$. However, this increase is not sustained due to the dependence of the power output on the flow rate through the hydraulic motor ($U_{\text{plm}}$). At higher values of $R_{\text{gen}}$, when there is a higher resistance to the flow through the motor, $U_{\text{plm}}$ decreases since $U_{\text{plm}} = P_{\text{load}}/R_{\text{gen}}$, and since the power output also appears to have a direct proportionality to the square of $U_{\text{plm}}$, it decreases. Thus, the power output varies non-monotonically with $R_{\text{gen}}$, and the optimal $R_{\text{gen}}$ that maximizes the power output is a compromise between these two factors.

In order to determine the optimal generator resistance, we perform simulations at different cycle heat-source temperatures and with a selection of working fluids (n-pentane, water, ammonia and R245fa), over a range of $R_{\text{gen}}$ values. In Fig. 5a and b the oscillating frequency and power output, respectively, are plotted as functions of $R_{\text{gen}}$ for four working fluids at a heat-source temperature of 200°C. In addition, power outputs when using different heat-source temperatures are plotted in Fig. 5c. For some working fluids and at lower heat-source temperatures (e.g., water at 200°C and pentane at 100°C), there are no sustained oscillations in the engine due to the very low flow rates caused by the high generator resistances ($R_{\text{gen}} > 5 \times 10^9$ kg m$^{-2}$ s$^{-1}$).

From the figures, it can be seen that the oscillating frequency remains largely invariant to the generator resistance, whereas the power output is strongly affected by the value of $R_{\text{gen}}$. As expected, the power output is almost negligible at low values of $R_{\text{gen}}(< 10^8$ kg m$^{-2}$ s$^{-1}$) and also at high values of $R_{\text{gen}}(> 10^9$ kg m$^{-2}$ s$^{-1}$). The power output peaks in the range $2 \times 10^7$ kg m$^{-2}$ s$^{-1}$ to $7 \times 10^7$ kg m$^{-2}$ s$^{-1}$, irrespective of the working fluid employed or the heat-source temperature. For most of the simulations, the maximum power is generated at a value of $R_{\text{gen}} = 5.6 \times 10^7$ kg m$^{-2}$ s$^{-1}$, and thus this value of $R_{\text{gen}}$ is employed as the optimal value for the subsequent simulations in this work.

For a few of the working fluids, e.g., some siloxanes, the optimal $R_{\text{gen}}$ differs from the above value, but only slightly, usually in the range of $\pm 5\%$. The optimal value of $R_{\text{gen}}$ is therefore generally insensitive to the choice of the working fluid but mainly a function of the engine configuration and component sizes. Thus, it should be noted that the selection of the optimal $R_{\text{gen}}$ is key in designing an optimal engine configuration and, as such, the designer should ensure the right value is selected for the engine configuration and imposed external conditions.
3. Thermodynamic property characterization of the Up-THERM engine

Having characterized the optimal configuration of the Up-THERM heat engine with respect to the imposed external conditions, it is of interest to investigate the performance of the engine with various working fluids, and to attempt to characterize the engine’s performance in relation to the thermodynamic properties of suitable working fluids. This can enable a determination of the properties that have the most significant effects on the engine performance and aid in the screening of working fluids in future selection processes; similarly to what was attempted for another TFO device (the NIFTE) by Markides et al. [35].

In order to determine the most-important thermodynamic properties, we carry out a parametric investigation on the engine’s exergy efficiency and power output where each thermodynamic property (or property combination) is varied separately and independently while the others are set to their nominal values at the nominal saturation temperature. The independent properties investigated are the: saturation temperature ($T_{sat}$); entropy change during vaporization ($\Delta s_v$); vapour-phase heat-capacity ratio ($\gamma_v$); vapour-phase density ($\rho_v$); liquid-phase density ($\rho_l$); and saturation pressure ($P_{sat}$). The enthalpy change during vaporization ($h_g$) and volume change during vaporization ($\nu_g$), although dependent on $T_{sat}$ & $T_{lg}$ and $\rho_g$ & $\rho_l$ respectively, are also investigated in the first instance.

Water is used as the reference working fluid here, due to its larger thermodynamic property variations, e.g., in $h_g$ and $\Delta s_v$ over organic fluids. The nominal point is set at an equilibrium/saturation temperature of 185 °C, which corresponds to heat-source and heatsink temperatures (from Eq. (23)) of 360 °C and 10 °C respectively. The nominal values of the investigated thermodynamic properties are thus calculated at 185 °C. $T_{sat}$ is varied from 20 °C through the nominal point to the critical temperature. The values of $\Delta s_v$, $h_g$, and $\nu_g$ generally decrease with increasing $T_{sat}$, becoming zero at the critical temperature. The liquid-phase density $\rho_l$ also decreases with increasing $T_{sat}$, but at the critical temperature it becomes equal to $\rho_g$, which increases with $T_{sat}$. Both $P_{sat}$ and $\gamma_v$ also increase with increasing $T_{sat}$, with $\gamma_v$ increasing very rapidly closer to the critical temperature. These trends are illustrated in Fig. 6.

3.1. Individual thermodynamic property variations

The results of varying each of the aforementioned thermodynamic properties independently are presented in Fig. 7. The oscillating frequency $f$ is generally insensitive to these variations with increasing $q$, to $c_176$, and the heat-source temperature $q_{gen}$ from 200 °C.

Fig. 5. Up-THERM engine performance as a function of generator resistance ($R_{gen}$): (a) Engine oscillating frequency ($f$) with four working fluids and heat-source temperature of 200 °C. (b) Engine power output ($P-W$) with four working fluids and heat-source temperature of 200 °C. (c) Engine power output ($P-W$) with four working fluids and various heat-source temperatures.

Fig. 6. Variations in normalized working-fluid thermodynamic properties ($X_{lg}$)—entropy change during vaporization ($\Delta s_v$), enthalpy change during vaporization ($h_g$), volume change during vaporization ($\nu_g$), liquid-phase density ($\rho_l$), vapour-phase density ($\rho_v$), liquid-phase density ($\rho_l$), and saturation pressure ($P_{sat}$)—with saturation temperature ($T_{sat}$) for water as the working fluid. Each thermodynamic property is normalized between 0 and 1 using the formula $X_{lg} = (X - X_{min})/(X_{max} - X_{min})$, where $X$ represents any of the aforementioned thermodynamic properties.

(Fig. 7a), although deviations from the nominal frequency can be seen with changes to the volume change during vaporization $\nu_g$ and saturation pressure $P_{sat}$. The increase in $f$ at higher (and slight decrease at lower) $P_{sat}$ is to be expected as larger pressures correspond to larger driving forces, generating more-frequent oscillations (and vice versa).

The influence of the thermodynamic properties on the exergy efficiency $\eta_{ex}$ and the power output $P = W$ are presented in Fig. 7b and 7c. Amongst the independent properties, $P_{sat}$ and $\rho_g$ have the greatest combined effect on the exergy efficiency and power output from the Up-THERM engine. The volume and entropy changes during vaporization, $\nu_g$ and $\Delta s_v$, and the saturation temperature $T_{sat}$ also have some effect on these indices, while $\Delta s_v$ and $h_g$ are less-important properties in affecting performance in this analysis. The fact that $T_{sat}$ has only a slight effect on the engine performance (the power output decreases slightly as $T_{sat}$ is increased) may suggest that it is not a key thermodynamic property with respect to power output and exergy efficiency. It does however play a key role in the initial screening and selection of working fluids as detailed in Section 4.1.

In particular, $\nu_g$ (a function of $\rho_g$ and $\rho_l$), is seen to have a profound effect on the exergy efficiency, especially at low saturation temperatures (corresponding to higher values of $\nu_g$; see Fig. 6).
Also, high values of \( v_{fg} \) (at low \( T_{sat} \)) lead to very low power outputs from the engine, in contrast to the fact that higher oscillating frequencies are experienced at these high values. When \( v_{fg} \) is large, there is a larger volume of working-fluid vapour generated during evaporation over the hot heat-exchanger per unit heat (and exergy) input, which translates to increased positive-displacement work per unit heat input, i.e., higher efficiency such as seen in Fig. 7b. At the same time, the heat/exergy input to the engine is very low, which eventually translates to reduced power outputs.

From Fig. 7c, the engine is seen to produce higher power outputs at low values of \( \rho_{g} \) (at low \( T_{sat} \)) and to produce lower power outputs at higher values. This can be attributed to the influence of these properties on the thermal resistance \( R_{th} \). Referring to Eq. (10), \( P_{sat} \) varies directly with \( \rho_{g} \) and \( T_{sat} \); thus low values of \( \rho_{g} \) and \( T_{sat} \) lead to low thermal resistances, which enable more heat to be exchanged between the working fluid and the heat exchangers. This eventually makes more thermal energy available for subsequent conversion to power in the load arrangement. Similarly at low values of \( s_{fg} \) (corresponding to high \( T_{sat} \)), a lower thermal resistance is experienced leading to higher power outputs from the engine.

The saturation pressure \( P_{sat} \) has the greatest influence of all varied properties on the power output in Fig. 7c. The power output increases with \( P_{sat} \) from low values to values above the nominal, beyond which a maximum is observed at a pressure of 69.6 bar (corresponding to a reduced pressure and temperature of 0.315 and 0.863 respectively). While \( \rho_{g} \) is equally important, it has an opposite effect to that of \( P_{sat} \). Higher values of \( P_{sat} \) lead to higher power outputs, while lower values of \( \rho_{g} \) also lead to higher power outputs. For any single working fluid, it is almost impossible to simultaneously achieve a high value of \( P_{sat} \) and a low value of \( \rho_{g} \) since both properties increase (or decrease) with increasing (or decreasing) \( T_{sat} \). Therefore, in most cases a compromise has to be reached between these properties; this relationship is further explored in the next subsection by simultaneously varying groups of thermodynamic properties.

### 3.2. Combined thermodynamic property variations

In the previous section, the saturation pressure \( P_{sat} \) and the vapour-phase density \( \rho_{g} \) were identified as very significant properties in describing the Up-THERM engine performance. We now vary combinations of (two, three and four) properties to investigate any synergies that may exist between property groups and to also identify which of \( P_{sat} \) or \( \rho_{g} \) is more important in affecting performance. The resulting performance predictions are presented in Fig. 8 for the exergy efficiency and Fig. 9 for the power output. Some combined variations (e.g., of \( s_{fg} \) and \( \gamma_{fg} \)) result in higher efficiencies and/or power outputs over the individual properties.

From the results, the key role of varying \( P_{sat} \) in affecting performance persists when it is varied in combination with other properties. In particular, the simultaneous variation of \( P_{sat} \) and \( s_{fg} \) has a stronger effect on both the power output and exergy efficiency than varying \( P_{sat} \) alone. Efficiency and power output (up to a point) are both seen to increase with the combination of high \( P_{sat} \) and low \( s_{fg} \). Interestingly, however, the combination of high \( P_{sat} \) and \( T_{sat} \) causes a reduction in power output from that previously attained at higher \( P_{sat} \) alone. Thus a combination of high saturation pressures and low equilibrium/saturation temperatures is needed to maximize power output from the engine. This suggests that one needs a fluid with as high a \( P_{sat} \) as possible at any corresponding \( T_{sat} \) to maximize the power output.

Similarly, the performance trends in the variations of \( \rho_{g} \) are seen to persist when other thermodynamic properties are
Fig. 8. Exergy efficiency ($\eta_{\text{ex}}$) of the Up-THERM heat engine with water as the working fluid on varying combinations of its thermodynamic properties (see legends for combinations). Each property combination is varied between the indicated saturation temperature ($T_{\text{sat}}$) range while others are set to their respective nominal values at a saturation temperature of 185 °C.

Fig. 9. Power output ($P$) from the Up-THERM heat engine with water as the working fluid on varying combinations of its thermodynamic properties (see legends for combinations). Each property combination is varied between the indicated saturation temperature ($T_{\text{sat}}$) range while others are set to their respective nominal values at a saturation temperature of 185 °C.
simultaneously varied. As expected, the improvements on performance due to simultaneous variations of $T_{\text{sat}}$ and $\rho_6$ or $\gamma_{\text{fg}}$ and $\rho_6$ are insignificant compared to those of varying $\rho_6$ alone. There is, however, a slight increase in power output at combinations of low $\rho_6$ and low $T_{\text{sat}}$.

The simultaneous variation of combinations of $P_{\text{sat}}$ and $\rho_6$ is seen to result in very different trends from those obtained when these properties are varied individually. In fact, variation in each property tends to nullify the effect of the other on the power output; they do, however, reinforce each other in terms of the exergy efficiency, with $\eta_{\text{ex}}$ increasing rapidly from the nominal value at lower values of $\rho_6$ and $P_{\text{sat}}$. Thus, for a high-power design one needs a combination of a high $P_{\text{sat}}$ and high $\rho_6$ fluid (low $\rho_6$ should be avoided), whereas for a high-efficiency design a combination of low $\rho_6$ and low $P_{\text{sat}}$ is needed. In order to simultaneously attain a high power output and a high exergy efficiency one needs a combination of high $P_{\text{sat}}$ and low $\rho_6$, which is not physically realizable for most known fluids as both $P_{\text{sat}}$ and $\rho_6$ increase with $T_{\text{sat}}$. This suggests that power output and efficiency are competing performance objectives; high-power designs will generally have lower exergy efficiencies and vice versa.

The simultaneous variation of combinations of three or four properties serve to further confirm the earlier findings, since the general trends (in variations of $P_{\text{sat}}$ and $\rho_6$) from both the single-property and two-property variations are found to persist when three or more properties are varied simultaneously. When either $T_{\text{sat}}$, $\gamma_{\text{fg}}$ or $s_{\text{fg}}$ are varied in combination with $P_{\text{sat}}$ and $\rho_6$ the previous trends in power and efficiency persist, especially the sharp increase in efficiency below the nominal point. This supports the earlier inference of the competition between power output and exergy efficiency, and further highlights the conflicting importance of $\rho_6$ and $P_{\text{sat}}$. The identification of these key combinations of thermodynamic properties is particularly important and informative for the computer-aided molecular design (CAMD) of these engines.

### 3.3. Comparison with an ideal two-phase and other thermofluidic devices

As earlier stated, the Up-THERM engine and the Non-Inertive-Feedback Thermofluidic Engine (NIFTE), both belong to the same class of two-phase oscillatory heat engines known as thermofluidic oscillators. These two-phase engines in general can be characterised by a working fluid thermal efficiency, $\eta_{\text{th}}$. This is a theoretical ideal thermal efficiency relating to the useful work done in transferring a working fluid across two constant-pressure (and temperature) reservoirs, employing only positive-displacement phase-change processes and ignoring any exergy destruction via valves and thermal losses [35]. This generally characterises any two-phase heat engine as no information about the physical engine (Up-THERM or NIFTE or otherwise) is required in its definition. A working fluid exergy efficiency $\eta_{\text{ex},\text{th}}$ can be further defined by dividing $\eta_{\text{ex}}$ by the Carnot efficiency corresponding to the hot and cold temperature reservoirs.

An investigation of the effect of working fluids and their thermodynamic properties on $\eta_{\text{ex}}$ was carried out by Markides et al. [35], to highlight the working fluids with the highest potential to convert heat to work in any two-phase heat engine. They found that $\eta_{\text{ex}}$ generally increases with the heat-addition temperature irrespective of the working-fluid employed, as expected. However, its exergetic component, $\eta_{\text{ex},\text{th}}$, decreases with heat-addition temperature. Also, the organic working fluids (pentane and R245ca) were seen to exhibit higher $\eta_{\text{ex},\text{th}}$ and lower $\eta_{\text{ex}}$ in comparison to the hydrogen-bonding fluids (water and ammonia) at the same reduced temperatures. Furthermore, amongst the working-fluid properties, the volume change during vaporization ($v_{\text{g}}$) had the strongest effect on $\eta_{\text{ex}}$ with $\eta_{\text{ex}}$ decreasing with decreasing $v_{\text{g}}$ (increasing $T_{\text{sat}}$). The saturation pressure ($P_{\text{sat}}$) leads to the second-largest deviation, with $\eta_{\text{ex}}$ increasing with $P_{\text{sat}}$. Other thermodynamic properties had less significant effects on the working fluid efficiencies.

These results are replicated in both the NIFTE and the Up-THERM where changes in $v_{\text{g}}$ have the greatest influence on the exergetic efficiencies of both devices. In the Up-THERM, the exergy efficiency decreases with decreasing $v_{\text{g}}$. In the NIFTE however, the exergy efficiency increases with decreasing $v_{\text{g}}$ in the first instance, until a maximum and then decreases [35]. $P_{\text{sat}}$ and the entropy change during vaporization ($s_{\text{fg}}$) are also seen to have significant effects on the exergy efficiency of the Up-THERM and its power output. In addition, thermodynamic properties such as the liquid-phase density ($\rho_6$), the vapour-phase heat-capacity ratio ($\gamma_{\text{fg}}$) and the saturation temperature ($T_{\text{sat}}$) are seen to have less significant effects on the exergy efficiencies of both the NIFTE and the Up-THERM engines. Finally, while the effect of the vapour-phase density ($\rho_6$) on the working fluid efficiency and the exergy efficiency of the NIFTE was not reported, it is seen to have significant effects on the efficiencies and power output of the Up-THERM.

### 4. Working-fluid selection for the Up-THERM engine

#### 4.1. Available working fluids

Currently, there are a number of publications on working-fluid selection for different heat engines, especially for the ORC variants. It is generally accepted that it is challenging to select an optimal working fluid for all cycle configurations, operating conditions and heat-source temperatures, which makes it difficult to generalize working-fluid selection rules across different cycles. Chen et al. [49], in an investigation of 35 pure working fluids (refrigerants, hydrocarbons and ammonia) in ORCs, suggested that the critical temperature and the slope of the saturated vapour curve (on a $T$–$s$ diagram) of working fluids are important characteristics to consider when designing cycles and selecting operating conditions. Furthermore, siloxanes (MM, MDM, MD2M, MD3M and MD4M) have been investigated as suitable working fluids for medium- and high-temperature cycles [10,50].

Various other factors influence the selection of (organic) working fluids, including the stability, material compatibility, safety, environmental impact and purchase cost of the prospective fluids. Organic working fluids are known to suffer chemical and physical deterioration at high temperatures, thus the stability of the fluid at the maximum temperature in the cycle should be considered before selection. The selected working fluid should also be non-corrosive and compatible with the engine materials and lubricants. Various authors [51–55] have presented techniques for studying the thermal and chemical stability of various refrigerant-fluid systems. It is also important to ensure that the selected fluid has a negligible environmental imprint in terms of its ozone-depletion potential (ODP), atmospheric lifetime and global-warming potential (GWP). Refrigerants such as R-11, R-12, R-113, R-114, and R-115 have been phased out while others such as R-21, R-22, R-123, R-124, R-141b and R-142b are in the process of being phased out due to their detrimental environmental impact [49]. A few of these fluids are considered in this work for comparison purposes.

The working fluids considered in this work are listed in Table 3, and include hydrocarbons (straight-chain alkanes, branched alkanes and aromatics), water and ammonia, refrigerants (halogenated alkanes) and siloxanes. The properties of these fluids are taken from the NIST database [56], which contains experimentally validated data of various fluids. Other approaches for providing
working-fluid thermodynamic property values do exist, notably from a molecular perspective including the statistical associating fluid theory (SAFT) equations of state (EoS) [79,12,57–61]. While these EoS have been demonstrated to predict accurately the thermodynamic properties of relevant fluid systems, current databases are not yet exhaustive, and since the NIST database contains a larger set of fluids, it is preferred for the purposes of the present study. The molecular-based EoS will however play an important role in the computer-aided molecular design (CAMD) of working fluids for waste-heat recovery systems in general [62] and the Up-THERM heat engine in particular.

For a two-phase thermofluidic-oscillator engine like the Up-THERM, it is important that the working fluid be able to undergo phase change at the externally imposed cycle temperatures. This makes the critical temperature of the working fluid a very important thermodynamic selection criterion. Specifically, the equilibrium temperature of the engine (which corresponds to the mean saturation temperature of the working fluid) should be below the critical temperature of the working fluid \( T_C \) to ensure the formation of a vapour phase and present a significant phase change at the externally imposed cycle temperatures. This means between 1.5 Hz and 2 Hz with the refrigerant R113 having the lower frequencies than the lighter working fluids, such as the alkanes generally have high critical temperatures.

It can be seen that heavier alkanes with increasing chain lengths have progressively higher critical temperatures, and that the siloxanes generally have high critical temperatures. One of the more apparent inferences from Fig. 11 is the link between the power output (and/or efficiency) and the saturation temperature of the engine with the different working fluids arranged in oscillating frequency and the operating pressure (saturation pressure) of the engine with the different working fluids arranged in decreasing magnitude of power output are shown, while a plot of the power output against the exergy efficiency of the engine for a given working fluid is shown in Fig. 11b.

Using the properties of these fluids, the Up-THERM engine model is simulated with the nominal heat source/sink conditions and all other system parameters (e.g., related to the geometry/size of the device) kept constant. The results of these simulations are presented in Fig. 11; in Fig. 11a the resulting thermal efficiency, oscillating frequency and the operating pressure (saturation pressure) of the engine with the different working fluids arranged in decreasing magnitude of power output are shown, while a plot of the power output against the exergy efficiency of the engine for a given working fluid is shown in Fig. 11b.

When using the different pre-selected working fluids, the operating/oscillating frequency of the Up-THERM engine varies between 1.5 Hz and 2 Hz with the refrigerant R113 having the lowest frequency and none of the highest one. Also, the higher-molecular-weight fluids, such as the siloxanes, are seen to exhibit lower frequencies than the lighter working fluids, such as the alkanes. Overall, the oscillating frequency is not strongly affected by the choice of working fluid. Also, it is noted that in this analysis the exergy efficiency and the thermal efficiency are, in fact, proportional and will show identical trends, since the heat source and sink temperatures (and therefore, the Carnot efficiency in Eq. (22)) are the same.

One of the more apparent inferences from Fig. 11a is the link between the power output (and/or efficiency) and the saturation
pressure. While all the working fluids are operating at the same equilibrium/time-mean saturation temperature of 185 °C, they will have different saturation pressures based on their vapour–liquid equilibrium curves. There is a strong positive correlation between $P_{\text{sat}}$ and the power output and a negative correlation between $P_{\text{sat}}$ and the exergy and thermal efficiencies; the fluids with higher $P_{\text{sat}}$, such as R113 and the hexanes, have higher power outputs and lower efficiencies than the fluids with lower $P_{\text{sat}}$, such as decane and MD4M. This, a competition arises between the engine's power output and its exergy and/or thermal efficiency, which appear as conflicting design objectives.

An obvious trend from Fig. 11b is the inverse and multi-objective relationship between the power output from the Up-THERM engine and its exergy efficiency; working fluids with a high power output have a low efficiency, and vice versa. This follows from the results in Fig. 11a and Section 3, where higher working-fluid saturation pressures are associated with higher power outputs, while lower values of vapour-phase density $\rho_g$ lead to higher power outputs and higher exergy efficiencies. As these two thermodynamic properties both vary directly with the saturation temperature $T_{\text{sat}}$, both scenarios (high $P_{\text{sat}}$ and low $\rho_g$) cannot be simultaneously achieved. The working fluids that lead to high-power engine designs are R113, $i$-hexane and $n$-hexane with correspondingly low exergy/thermal efficiencies. Similarly, the working fluids that lead to high-efficiency engine designs are the siloxanes in general, decane and nonane with correspondingly low power outputs. The existence of an inverse relationship between power output and efficiency confirms the earlier inference that one cannot simultaneously achieve high-power and high-efficiency engine designs.

It is also important to highlight the performance of the engine within and amongst the chemical classes of working fluids present. Most of the applicable screened fluids are dry fluids; only water is a wet fluid and the aromatic compounds (benzene and toluene) are the only isentropic fluids (see Table 3). It is interestingly the case that the dry fluids dominate the results in Fig. 11: dry fluids lead to the engines with the highest power output (R113 and the hexane isomers) and also to the highest efficiencies (the siloxanes). This conclusion may, however, not be applicable at lower heat-source temperatures as more working fluids become ‘feasible’ as discussed in Section 4.3. Furthermore, within a particular chemical class of working fluids, e.g., the straight-chain alkanes, the shorter-chain and lighter-molecular-weight compounds result in designs with higher power outputs (and lower efficiencies) while the longer-chain and heavier compounds result in higher efficiencies (and lower power outputs). This is exemplified by the alkanes and the siloxanes. Engines with fluids from $n$-hexane, $n$-heptane to $n$-decane progressively have lower power outputs and higher efficiencies. Similarly, from MM to MD4M and from D4 to D6, the fluids progressively display higher efficiencies and lower power outputs. This suggests that the power output and the efficiencies correlate negatively and positively respectively with the molecular weight of the working fluids. As the critical properties ($T_c$ and $P_c$) are related to the molecular weights as seen in Fig. 10—within a chemical class, e.g., the alkanes or siloxanes, heavier compounds have lower $P_c$ and higher $T_c$ and vice versa—the performance of the engine may also be dependent on the critical properties of the working fluids; this is investigated in Section 4.4.

The performance of the engine with $n$-hexane and $i$-hexane as working fluids also reveals a reciprocal relationship between isomers. The branched alkane ($i$-hexane in this case) results in a higher power output and slightly lower efficiency than the straight-chain alkane. The branched alkane could be interpreted as behaving like its corresponding lighter alkane, exhibiting a higher power output and a lower efficiency. This relation is further encountered in Section 4.3 when more isomer pairs are considered. Also, between the aromatic compounds, the substitution of the hydrogen atom in benzene with the methyl group in toluene (the heavier compound) results in an engine with a lower power output and higher efficiencies. Furthermore, a closer inspection of Fig. 11 reveals that the compounds with higher molecular weights, especially the siloxanes, are concentrated on the high-efficiency (and low-power-output) end of the graph while those with lower molecular weights are concentrated on the high-power end of the graph. This highlights the compromise necessary between the power output and the efficiency with molecular weight.

### 4.3 Working fluids for varying heat-source temperature

In Sections 3 and 4.2 we established the challenge inherent in selecting working fluids to simultaneously maximize both the power output and efficiency of the Up-THERM engine. In this section, we investigate and concentrate on working-fluid selections for off-design conditions at different heat-source temperatures. In Fig. 12, we present the performance of various working fluids...
when used with the engine at lower heat-source temperatures of 100 °C and 200 °C. Similarly, in Fig. 13 results are presented for heat-source temperatures of 300 °C and 400 °C. In both sets of figures, the working fluids are arranged in order of decreasing engine power output. These simulations were all carried out with a heat-sink temperature of 10 °C, as before.

The investigated working fluids are once again taken from Table 3. At the lower heat-source temperatures of 100 °C and 200 °C, more fluids become available for consideration as more refrigerants now have critical temperatures above these equilibrium temperatures, enabling the necessary two-phase flow in the device. Also available for consideration are the lighter hydrocarbons such as pentane and butane, and ammonia. At the higher heat-source temperature of 400 °C, working fluids such as R113 and i-hexane become excluded from consideration as the equilibrium temperature is now greater than their critical temperatures.

Most of the findings from the nominal-design case with heat-source temperature of 360 °C are replicated at heat-source temperatures from 100 °C to 400 °C as shown in Figs. 12 and 13. Fluids with higher equilibrium saturation pressures are seen to produce higher power outputs (with lower efficiencies), while those with lower saturation pressures produce lower power outputs. Also, within the alkane homologous series the lighter compounds produce higher power output and lower exergy/thermal efficiencies than the heavier compounds, highlighting the respective positive and negative correlation of efficiency and power output with molecular weight. The oscillating frequency remains largely unaffected by the choice of working fluid.

As observed earlier with the hexane isomers, the performance of the engine with butane isomers also exhibits a reciprocal relationship. From Fig. 12, the branched alkane (i-butane in this case) results in a higher power output and slightly lower efficiency than the straight-chained alkane (n-butane). This is also observed with i-hexane and n-hexane at higher heat-source temperatures. Also interesting here is the comparison between saturated and unsaturated alkanes (C3H8 and C3H6 respectively) at the low heat-source temperature of 100 °C. The alkene results in a higher power output (and slightly lower efficiencies) than the alkane, agreeing with an expectation based on their respective molecular weights.

The availability of more working fluids at lower heat-source temperatures introduces a more interesting comparison amongst the chemical classes of working fluids present. A close inspection of Fig. 12 for the heat-source temperatures of 100 °C and 200 °C reveals that the wet fluids—R32, R143a, propene and ammonia—occupy the high power (and low efficiency) end of the figures, whereas the dry fluids occupy the high exergy-efficiency end of the figures; this is quite different from the result in Figs. 11 and 13 where the dry fluids are dominant. This finding is, however, directly influenced and subject to the low critical temperatures of most of the wet fluids, which is why they were excluded by pre-screening at the high heat-source temperatures. These results suggest that, when available, wet fluids are more suitable for the high-power-output designs, while the dry fluids are more suitable to the high efficiency designs.

4.4. Effect of critical properties

In Section 3 it was concluded that the working-fluid (equilibrium) saturation pressure $P_{\text{sat}}$ and its (equilibrium) vapour-phase
density are important thermodynamic properties in controlling the performance of the Up-THERM heat engine. It was also established that the power output and exergy efficiency correlate strongly with $P_{\text{sat}}$ from Figs. 11–13. The molecular weight of working fluids also appeared to be significant in optimizing the engine output, especially within a homologous series of working fluids as in Section 4.2. These indicate that the critical properties of the fluid will play an important role in working-fluid selection and performance optimization of the Up-THERM engine.

Hence, we investigate here the relationship between the engine performance and the working-fluid critical properties. In particular, we compare the power output to the reduced and critical properties of the applicable working fluids, while minding the fact that the power output and the thermal/exergy efficiency are inversely correlated. This is done at heat-source temperatures of 200°C and 360°C and the results are presented in Figs. 14 and 15, respectively; the corresponding working fluids in these results are the same as those in Figs. 11 and 12. In these figures, the reduced pressure is defined as $P_r = \frac{P_{\text{sat}}}{P_c}$ and the reduced temperature is defined in a similar manner.

The correlation between the engine performance and the working-fluid critical properties is evident in both figures. From Fig. 14, the engine’s power output is seen to decrease as the working-fluid critical temperature increases. This of course implies that its thermal/exergy efficiency increases with the critical temperature. Since the equilibrium saturation temperature ($T_{\text{sat}} = (200 \times 10^2 - 300 \times 10^2)/2$) is the same across all the working fluids, it is indeed expected and not surprising that the engine’s power output will increase (while the efficiencies will decrease) with the working-fluid reduced temperature due to its definition. Thus, not only is the critical temperature $T_c$ important in the pre-screening process of excluding non-applicable working fluids at different heat-source temperatures as used in Fig. 10, it also has a telling impact on the power output and/or the efficiency of the engine. High-power designs will require working fluids with low (but still feasible) $T_c$ whereas high efficiency designs will require fluids with high $T_c$.

While the critical temperature clearly dictates working-fluid selection and the performance of the engine, the role of the critical pressure $P_c$ is less obvious, although higher critical pressures do tend generally to result in higher power outputs amongst working fluids from the same family. Also, while all working fluids have the same $T_{\text{sat}}$, they all have different saturation pressures $P_{\text{sat}}$ based on their vapour–liquid equilibrium (VLE) curves. The normalization of the working-fluid critical pressure based on the equilibrium saturation pressure in the definition of the reduced pressure $P_r$ does, however, result in a more definite trend with respect to the engine’s performance. In Fig. 14 it is clear that the engine’s power output increases as the reduced pressure increases. Conversely, high-efficiency designs will be favoured by low reduced pressures.

In summary, working fluids with low critical temperatures or high reduced temperatures and high reduced pressures can result in engines that will deliver a high power output. This is particularly well demonstrated by ammonia (see Fig. 10) at a heat-source temperature of 200°C in Fig. 12, which delivers more than double the power output of the closest neighbour, R236fa. This is further explored in the next section. In Fig. 15, the engine’s performance at a heat-source temperature of 360°C is presented against the working-fluid critical properties. Compared to Fig. 14 it does appear more scattered, but nevertheless, one arrives at the same
interpretations that can be generalized for different heat source/sink temperatures.

4.5. Optimal working-fluid selection

In Fig. 16a, the maximum power output from the Up-THERM heat engine over all working fluids is plotted against the corresponding heat-source temperature. The ‘optimal’ working fluid responsible for this maximum power output is also indicated at the different heat-source temperatures. As the heat-source temperature is varied, the optimal working-fluid changes, with R32 being optimal at 100 °C and hexane being optimal at 400 °C. Noticeable in this figure are the discontinuities as the heat-source temperature is varied. These are a result of the exclusion of working fluids when the condition $T_{\text{sat}} > 95^\circ C$ is imposed, as dictated by Fig. 10. A few of the optimal working fluids are seen to be very versatile especially at low heat-source temperatures, being optimal across large ranges of heat-source temperatures.

At heat-source temperatures below about 210 °C, it is found that the optimal working-fluids are predominantly wet fluids. This supports the earlier inference that, where applicable, Up-THERM designs with wet working-fluids produce higher power outputs (and correspondingly lower efficiencies). Ammonia in particular is the most versatile of the working fluids, being the optimal fluid between heat-source temperatures of 150 °C and 210 °C. This is a direct result of its low critical temperature and high critical pressure as highlighted in the previous section. At higher temperatures however, there are more frequent discontinuities in the optimal curve, with dry and isentropic working fluids being optimal between 215 °C and 300 °C while only dry fluids are feasible and optimal at higher heat-source temperatures.

Finally, Fig. 16a can be used as a working-fluid selection map for the Up-THERM engine. From this figure, an optimal working fluid can be selected as a function of the available heat source(s). A few of these fluids (those italicized in Table 3), especially at higher heat-source temperatures, are already or are soon to be phased out due to the Montreal protocol [63]. For this reason, a second map, Fig. 16b, is provided alongside the optimal map. This contains the working fluids that are second best in providing the maximum power output from the Up-THERM engine. These fluids can thus serve as second-best alternative substitutes for the phased out and soon to be phased out optimal working-fluids, where relevant.

4.6. Comparison with existing heat engines

At this stage, it is important to compare the Up-THERM engine with other established concepts in terms of both performance and economical viability. Suitable technologies for comparison at the relevant power output and heat-source temperature ranges are the organic Rankine cycle (ORC) and the Stirling engine, both of which already form the basis of known micro-CHP prime-mover systems [64,65]. ORC systems [7,8,10,50,61] are a relatively mature
technology capable of utilizing low-grade heat, while Stirling engines [26,28,29] are also able to utilise low-grade heat for subsequent conversion to electricity. ORCs are based on a conventional (two-phase) Rankine cycle but incorporating an organic working fluid, whereas Stirling engines are based on an inherently unsteady but single-phase thermodynamic cycle whereby the cyclic compression and expansion of a gaseous working fluid at different temperatures leads to a net conversion of thermal energy to mechanical work.

While the scope for comparison of these engines is quite wide, we will limit this discussion to engines with the same power output as the Up-THERM engine investigated in this work, i.e., in the 1 kW–10 kW range. A waste-heat recovery ORC engine operating on a refinery flue gas (at a source temperature of 330 °C), and delivering power output in excess of 10 kW is predicted to have a maximum thermal efficiency of about 15% [7]. Also, its specific investment cost (at power outputs between 1 kW and 10 kW) is predicted to range between €3000 and €7500 per kW of mechanical power produced. From the results in Figs. 11 and 13, it is clear that the high-power designs of the Up-THERM engine have thermal efficiencies between 5% and 12%. Although these thermal efficiencies are lower than those of ORCs above (about 15%), they have the same order of magnitude and are thus comparable. As discussed previously in Sections 4.2 and 4.3, the power output of the Up-THERM engine can be sacrificed in order to improve its efficiency; this can lead to Up-THERM engine designs with thermal efficiencies as high as those of ORC and Stirling engines, although in the opinion of the authors this is not a desirable goal overall.

Furthermore, it is envisaged that the Up-THERM engine will be much more affordable than ORC and Stirling engines due to its simple construction and operation, and small number of moving parts and dynamic seals – the Up-THERM contains only a single moving part, its solid reciprocating piston. Such single-piston engines have a number of advantages when compared to state-of-the-art Stirling engines, namely simplicity, adequate high-temperature sealing, elimination of heat losses, very low leakage rates and much easier balancing [39]. These, amongst others, will allow lower capital and operating costs for the Up-THERM engine with longer operating lifetimes. In addition, prototypes similar to the Up-THERM engine have been developed at costs of €200–€500 per kW of power generated; these are much cheaper than €2500–€4500 per kW for Stirling-type engines [41].

Thus, the Up-THERM engine can be said to offer an economically and technologically viable alternative to ORCs and Stirling engines in waste-heat recovery, solar, and combined heat and power (CHP) applications, especially for small-scale power generation in remote and/or off-grid locations.

5. Conclusions

A synopsis of a non-linear lumped dynamic model for a novel two-phase thermofluidic oscillator heat engine named Up-THERM has been presented (full details are provided in Kirmse et al. [37]). This engine relies on the periodic evaporation and condensation of its working fluid and the vertical motion of a single solid piston. The oscillatory motion of the piston and working fluid are transformed to a unidirectional flow of the working fluid through a hydraulic motor to extract power. With its few moving parts and dynamic seals, the resulting device is associated with low capital and maintenance costs. While the engine is specifically conceived for heat-recovery applications, it is generally relevant in low-power applications especially in remote or off-grid locations where low investment and maintenance costs are crucial for favourable returns, and economic viability.

The performance of the Up-THERM engine is defined here in terms of its exergy/thermal efficiency and its power output. In its nominal configuration with water as the working fluid and a heat-source temperature of 360 °C, the Up-THERM engine delivers 2.64 kW at an exergy efficiency of 11.2%. This can be compared with the nominal exergy efficiency of a similar device known as the NIFTE, which was reported by Markides et al. [35] as being of the order of 1%, and the maximum exergy efficiency value of 6% attained by varying working fluids but with a nominal geometric NIFTE design, although it is noted that the target heat-source temperatures in the case of the NIFTE are lower (<200 °C). However, the performance of the Up-THERM engine (at this nominal configuration) can be considerably improved by employing organic working fluids such as R113 and isomers of hexane, delivering up to 8 kW of power. The Up-THERM converter is also shown to offer an economically and technologically viable alternative to established technologies such as ORCs and Stirling engines in waste-heat recovery, solar and CHP applications, especially for small-scale power generation in remote and/or off-grid locations.

A key element of the Up-THERM engine’s design is the specification of the generator mounted to the hydraulic motor. The generator is characterized by its resistance, $R_{\text{gen}}$, with its value determined empirically as the one that maximizes power output. Simulations revealed that the power output varies over orders of magnitude with respect to this resistance, making its determination very important in characterizing the engine. The optimal value of $R_{\text{gen}}$ is however found to be generally insensitive to the external conditions of heat-source and heat-sink temperatures, and the employed working fluid.
The effects of several working-fluid thermodynamic properties on the performance of the engine were investigated. This was carried out using water as the reference working fluid at a nominal engine design, by varying combinations of the respective properties as functions of the saturation temperature $T_{sat}$, which revealed that the saturation pressure $P_{sat}$ and the vapour-phase density $\rho_v$ are the most dominant independent thermodynamic properties in terms of their effects on the power output and exergy efficiency of the engine. The entropy change during vaporization $s_g$ also has a marginal effect on the engine’s performance. Higher values of $P_{sat}$ and lower values of $\rho_v$ lead to higher power outputs. This particular combination of $P_{sat}$ and $\rho_v$ is virtually impossible for real working fluids as both properties increase (or decrease) with increasing (or decreasing) $T_{sat}$, suggesting a compromise has to be reached between both properties.

An important aspect of this work concerns the working-fluid selection for the Up-THERM engine. Due to its nature as a two-phase engine, it is important that the employed working fluid is capable of generating two-phase flow at the combinations of the heat-source and heat-sink temperatures. Only fluids with critical temperatures higher than the resulting equilibrium temperature will satisfy this condition. At the nominal design, R113 and i-hexane are the most promising fluids in furnishing a high-power-output engine, delivering more than double the output compared with water as working fluid. These fluids do, however, lead to low-efficiency designs as the engine’s efficiency and power output were found to be inversely related. Siloxanes and higher members of the alkane family result in high-efficiency engine designs, however with much lower power output.

A total of 46 working fluids including aliphatic and aromatic hydrocarbons, refrigerants and siloxanes were considered for use in the Up-THERM engine. Simulations with these fluids at various external (heat source) conditions revealed that the critical properties of the fluids have a profound effect on the engine’s performance. High-power designs were generally favoured by working fluids with low critical temperatures; the critical temperatures still need to be greater than the equilibrium temperature for feasible designs. Furthermore, working fluids with high reduced temperatures and pressures also favour high-power designs. Conversely, fluids with high critical temperatures and low reduced temperatures/pressure will favour high-efficiency engine designs. Thus, in a chemical family such as the alkanes, lower-molecular-weight members will favour high-power designs while heavier members will favour high-efficiency designs.

Finally, an optimal working-fluid selection map is presented in Fig. 16. This figure contains the working fluid(s) that maximize the engine’s power output at different heat-source temperatures. From this map, the engine is seen to deliver power output in excess of 10 kW especially at higher heat-source temperatures. Wet fluids were found to be optimal at heat-source temperatures below 210 ºC, and dry fluids were optimal at higher heat-source temperatures. Working fluids such as ammonia (in particular, owing to its low critical temperature and high critical pressure), R245ca, R32, propene and butane feature prominently on this map, generating high power-outputs over large heat-source temperatures ranges. This makes them suitable and adaptable to variations in heat-source and heat-sink temperatures while the engine is in operation. These working fluids are therefore good candidates for the Up-THERM heat converter.

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