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Multi-objective optimization of organic Rankine cycle systems considering their dynamic performance

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**Abstract**

The Organic Rankine cycle system is a well-established technology for converting the waste heat from internal combustion engines into mechanical or electrical power. For a vehicle, due to the engine load changes during the driving cycle, the mass flow rate and temperature of the waste heat fluctuate rapidly over a broad range. This poses high requirements to the control of the organic Rankine cycle unit, in order to ensure safety, high efficiency, system compactness and long component lifetime. This paper presents a novel design method for organic Rankine cycle systems subject to highly fluctuating heat sources, ensuring safe and efficient operation. An integral optimization code developed in MATLAB®/Simulink® combining the design of the thermodynamic cycle, the system evaporator and the control system with a dynamic simulation model is presented. The multi-objective optimization maximizes the organic Rankine cycle net power output over a driving cycle of a heavy-duty truck, while minimizing the mass of the evaporator. The results indicate that, in order to ensure safe operation, the degree of superheating of the working fluid as well as the exhaust gas temperature leaving the evaporator at design conditions should be higher than what classical steady-state thermodynamic analyses suggest.

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1. Introduction

The transport sector is responsible for almost one quarter of the greenhouse gas emissions in Europe, of which 70% are caused by transport on road [1]. Especially in the last two decades, particular focus has been set on the development of more environmentally-friendly vehicle powertrains. For instance, electrical drives have been proposed, in particular for smaller vehicles like passenger cars [2]. The electrification of heavy-duty trucks, which cover approximately one third of the emissions of road transport, appears to be quite challenging, mainly because of the high energy density that the batteries should have and the lack of infrastructure for trucks supplied by overhead lines [3]. For these reasons, internal combustion engines are still a relevant option for the propulsion of heavy-duty vehicles, possibly fuelled by an increasing share of power-to-X fuels from renewable energy sources [4,5]. A considerable increase in efficiency of internal combustion engines can be achieved by recovering the energy that is wasted in the form of heat [6,7]. Organic Rankine cycle (ORC) power systems are a cost-effective technology to recover medium/low temperature heat and convert it into mechanical or electrical power. ORC systems have extensively been installed to recover the waste heat of stationary diesel engines, gas turbines and industrial facilities [8–10]. In the context of heavy-duty vehicles, the ORC technology has faced several technical challenges, which have hindered its commercialization so far [11–13]: i) the mass flow rate and temperature of the waste heat fluctuate rapidly over a vast range, leading to a complex design and inefficiencies during part-load operation; ii) safe operation must be ensured despite the large fluctuations in waste heat; iii) the installation of the ORC unit requires additional space and mass that need to be transported penalizing the vehicle loading capabilities and iv) the backpressure of the internal combustion engine needs to be minimized in order to keep a high engine efficiency. These requirements, combined with the goal of maximum ORC power output, result in a trade-off among multiple objectives. In this way, the design of the ORC unit for heavy-duty trucks consists of a complex inter-disciplinary optimization problem, which involves thermodynamic design, component design, part-load operation, system dynamics and control. Several authors optimized ORC units affected by a variable heat source combining the design and the off-design operation in the same global optimization routine. The fluctuations of waste heat...
were handled by using a quasi-steady state approach, where dynamic effects were neglected [14–16]. For example, Lecompte et al. [14] carried out a combined design and off-design optimization of an ORC unit recovering waste heat from a diesel engine by developing a grid of stationary off-design points and optimizing for minimum specific investment costs per unit average power output. The advantages of an integrated design and off-design optimization were also highlighted for waste heat recovery from a billet reheat furnace by Pili et al. [15]. Considerably different results in terms of degree of superheating and evaporation pressure at design point resulted from the integration of design and off-design in the optimization. Gomez-Alaez et al. [16] investigated the waste heat recovery with an ORC unit in a natural gas pipeline compression station. Because of the hourly variations of the operating conditions, an optimization was carried out to find the optimal ORC configuration that could ensure the maximum annual energy production. The best configuration could achieve a net average efficiency of 19%. Guillaume and Lemort [17] performed a techno-economic optimization of an ORC unit recovering heat from a heavy-duty vehicle. The optimization was carried out for several stationary operating points of the engine, which were weighted according to their frequency of occurrence. The average net power output was the objective function to be maximized. Different working fluids, expansion machines and cycle architectures were investigated. Ethanol was found to be the most appropriate fluid in combination with a screw expander and engine exhaust gas recirculation.

Especially for road transport, it can be beneficial to consider the mass and volume of the ORC system already in the design phase, since they strongly affect the economic feasibility of the ORC integration [12]. Some authors included the trade-off among the ORC net power output and the mass and volume of the ORC unit in the design optimization [18,19]. Macian et al. [18] optimized the ORC unit for maximum net power output and then discarded the options that did not satisfy the volume constraint of 0.2 m³. Water was compared to R245fa as working fluids. Their results suggested that water can achieve a higher power output at the expenses of a larger volume. Pili et al. [19] optimized an ORC unit for truck applications and looked at the impact of working fluid selection on the power-to-weight and power-to-volume ratios. Although acetone and ethanol could provide the largest power output, isobutene showed larger power-to-weight and power-to-volume ratios. Other authors suggested a more holistic approach based on a multi-objective optimization of the ORC unit, where a Pareto front of optimal solutions is attained [20–24]. In particular, Yang et al. [22] carried out a multi-objective optimization of an ORC unit recovering waste heat from a truck engine. The authors selected the net power output and the total investment costs as counteracting objective functions. Their results suggested that R245fa is the best working fluid considering both thermodynamic and economic aspects as well as safety. The authors highlighted the importance of considering the off-design performance of the ORC unit when the operating conditions of the internal combustion engine change. Rosset et al. [23] investigated the design of an ORC unit equipped with a radial-inflow turbine recovering waste heat from a passenger car engine. For this purpose, a constrained multi-objective optimization was carried out. The net power output and the heat exchange area were the objective functions to be, maximized and minimized, respectively. The authors found that the optimal cycle configuration and the working fluid depend on the available space.
in the vehicle. Working fluids with boiling point close to the heat sink temperature, high critical pressure and high molecular weight allowed for better performances. Imran et al. [25] performed a multi-objective optimization of an ORC unit recovering waste heat from the exhaust gas of a heavy-duty vehicle driven by a 13 L diesel engine. The optimization targets were the unit net power output (to be maximized) and the unit overall cost, mass and volume (to be minimized). Several working fluids were investigated, among which pentane showed the best performance, reaching 8.3 kW on average on a truck driving cycle at a condensation temperature of 40 °C. The system dynamics were neglected, and a quasi-steady state approach was used for the off-design operation. The results of Ref. [25] also indicated that there is a trade-off between the unit power output and the cost, mass and volume. Holik et al. [24] optimized the design of an ORC unit for heavy-duty diesel trucks by maximizing the net power output and minimizing the total heat exchanger surface area, although for fixed mass flow rate and temperature of the heat source. Their results suggested that ethanol is the best fluid.

Given the large and rapid fluctuations in mass flow rate and temperature of the waste heat from heavy-duty trucks during a driving cycle, the dynamic response of the ORC system significantly affects the ORC performance, and should carefully be considered in order to ensure safe operation and maximum net power output. Wei et al. [26] compared two different approaches for the dynamic modelling of the heat exchangers in ORC systems: the finite-volume and the moving boundary approach. Compared to experimental data, the moving boundary approach resulted in lower accuracy, but also shorter computational time compared to the finite-volume approach. Quoilin et al. [27] presented a dynamic model of a small-scale ORC unit recovering waste heat from an internal combustion engine, based on a finite-volume discretization of the heat exchangers. Three different control strategies were proposed and compared, reaching a maximum heat recovery efficiency of 6.6%. Casella et al. [28] developed and validated a dynamic model of a 150-kW high temperature ORC system (the heat source was in the range between 450 °C and 500 °C). The model was able to predict the behaviour of the ORC unit with a maximum error of 3% in all main thermodynamic variables (pressures and temperatures at the evaporator and condenser). A comparison between the finite-volume and the moving-boundary approach for the dynamic modelling of heat exchangers in ORC units was also carried out by Desideri et al. [29]. The moving boundary approach allowed a significant reduction of the simulation time while keeping a good agreement with the experimental data in terms of estimated expander power output. Shu et al. [30] compared the influence of the working fluid on the dynamic response characteristics of an ORC unit recovering waste heat. The authors found that the dynamic response drops for straight-chain alkanes when the critical temperature increases. A comprehensive dynamic characterization of a mini ORC was carried out by Zhang et al. [31], where the impact on the ORC performance of variations in mass flow rate of working fluid, heat source and cooling medium was studied. The results of the study suggested that the mass flow rate of the ORC pump has a significant impact on the ORC thermodynamic conditions, and should be the preferred manipulated variable. Despite the interest in dynamic modelling of ORC systems, only a very limited number of previous works considered the dynamic performance in the ORC design phase [32,33]. Pierobon et al. [32] focused on the waste heat recovery from an offshore oil platform and analyzed a posteriori the feasibility of different designs in terms of dynamic performance, excluding the designs that did not satisfy the required specifications. An integrated optimization including the working fluid selection and the dynamic performance was carried out by Tillmanns et al. [33], although the dynamic model of the system (first-order system) and the time behaviour of the heat source (sine wave) were strongly simplified and far from realistic conditions.

The literature review suggest that only limited aspects of the integration of ORC units in heavy-duty vehicles have been included in the design optimization procedure so far. No holistic approach that includes the complex trade-off among multiple objectives, such as maximum power output and minimum component mass, and other essential aspects of this application, such as dynamic performance and controller design, has been developed yet. This work presents a novel design approach that includes and integrates the thermodynamic design, the component design, the dynamics and the controller design in the same global optimization loop. In this way, an optimal and feasible design is achieved, ensuring optimal performance and safe operation. The multi-objective optimization problem is solved by using the genetic algorithm and numerical models developed in MATLAB®/Simulink®. This work is of great interest not only for the truck application but also for other applications affected by transient operation, such as road, maritime and aviation transport, offshore platforms, as well as remote areas on land with no access to interconnected power grids.

This paper is divided into five sections. The waste heat recovery system is presented in section 2, followed by the presentation of the multi-objective optimization routine in section 3. The results of the multi-objective optimization are illustrated and discussed in section 4, while an outline of the conclusions can be found in section 5.

2. Waste heat recovery with organic Rankine cycle power system

The present work investigates the waste heat recovery of the exhaust gas of a 450-hp 13 L turbocharged diesel engine installed in a heavy-duty truck. The exhaust gas data were provided by a truck manufacturer, and refer to a 45-min trip. The time behaviour of the mass flow rate and temperature of the exhaust gas is shown in Fig. 1a, whereas the profile duration curve is given in Fig. 1b. The original exhaust data are provided in the supplementary material of Ref. [34]. It can be seen in Fig. 1a that the mass flow rate of the exhaust gas fluctuates quite rapidly over a broad range between 0.05 kg/s and 0.517 kg/s, whereas the temperature shows a slower trend fluctuating between 270 °C and 334 °C. The profile duration curve in Fig. 1b shows that the distribution of the mass flow rate and temperature of the exhaust gas over time is uniform and no particular value occurs more often than others do. The available waste heat rate \( Q_{aw} \) can be determined by the following equation:

\[
Q_{aw} = \dot{m}_{eg} c_{p, eg} (T_{eg, in} - T_{eg, ref})
\]

where \( \dot{m}_{eg} \) is the mass flow rate, \( c_{p, eg} \) the specific heat at constant pressure, \( T_{eg, in} \) the inlet temperature and \( T_{eg, ref} \) the reference temperature of the exhaust gas (subscript ‘eg’). The specific heat at constant pressure \( c_{p, eg} \) is a function of the chemical composition of the exhaust gas, which depends in turn on the operating conditions of the truck internal combustion engine and the exhaust gas after-treatment system. Since this information is not available, \( c_{p, eg} \) is approximated by using the properties of air. The reference temperature of the exhaust gas \( T_{eg, ref} \) is set to the minimum temperature allowable for the exhaust gas to avoid corrosion of the exhaust pipes. A value of \( T_{eg, ref} = 100 \) °C is chosen based on literature [35,36]. Given these assumptions, the available waste heat rate \( Q_{aw} \).
fluctuates between 10 kW and 114 kW, with an average value of 51.6 kW.

The exhaust gas is taken as the heat source of the ORC unit. The ORC plant consists of a simple ORC system without recuperator, since the recuperator increases costs, mass, volume and complexity of the ORC system. The layout of the ORC unit is shown in Fig. 2. The pump forwards the working fluid from point 0 to point 1, where it is preheated, vaporized and superheated to point 2 by receiving heat from the exhaust gas. The vapour at point 2 is then expanded in a turbine to point 3, where it is condensed back to point 0 while rejecting heat to a cooling medium, which is typically air or water. The ORC system can be controlled by manipulating two variables: i) the mass flow rate of the pump \( m_{wf, p}\) (or correspondingly the pump rotational speed) and ii) the opening of the exhaust gas bypass valve \( VO\).

3. Multi-objective optimization routine

In this section, the novel integrated multi-objective approach for the design of the ORC unit is explained. The optimization routine uses the genetic algorithm available in the Global Optimization Toolbox of MATLAB® [37] to solve the multi-objective optimization problem. The settings for the optimizer are reported in Table 1. While most of the settings have been kept at the default values suggested by MATLAB®, the population size has been set to 70 to limit the computational time. The genetic algorithm repeatedly changes the decision variables in order to find a Pareto front that minimizes or maximizes the objective functions. A set of ten decision variables is used for the optimization as summarized in Table 2. The first five variables refer to the thermodynamic design of the ORC system, while the last five variables refer to the design of the ORC evaporator, which is used to assess the mass of this component and, most importantly, to assess the dynamic off-design performance of the ORC unit over the driving cycle. It is worth highlighting that, since the waste heat fluctuates over time, the most general case needs to include the exhaust gas mass flow rate and temperature at design point in the set of decision variables, as shown in Table 2. In fact, it is not known a priori whether the optimal design should be at the peak of the available waste heat, at the time-weighted average or at any other condition. The guess values of exhaust gas mass flow rate and temperature are used for the thermodynamic, component and controller design, and they are updated by the optimizer after each optimization loop until the objective functions reach the desired maximum or minimum. Two objective functions were selected to demonstrate the feasibility of the proposed approach: i) the net power output of the ORC unit, which has to be maximized and ii) the mass of the evaporator, which needs to be minimized. The mass of the ORC evaporator can also be considered as an indicator of its volume as well as of its cost, since the mass is connected to the amount of material needed for the manufacturing of the component.

The net power output \( P_{net}\) is defined as follows:

\[
P_{net} = \dot{m}_{wf} \left( h_{wf,T,in} - h_{wf,T,out} \right) \eta_{TG} + \dot{m}_{wf} \frac{\left( h_{wf,P,in} - h_{wf,P,out} \right)}{\eta_{PMI}}
\]

where \( \dot{m}_{wf}\) and \( h_{wf}\) are the mass flow rate and the specific enthalpy of the working fluid, respectively, and the subscripts ‘\( T\)’ and ‘\( P\)’ refer...
to the turbine and the pump, respectively. The subscripts ‘in’ and ‘out’ refer to the inlet and outlet, respectively. The efficiencies $\eta_{TG}$ and $\eta_{PMI}$ refer to the turbine and generator mechanical and electrical efficiency and combined pump, motor and inverter mechanical and electrical efficiency, respectively. The mass of the evaporator $M_w$ is calculated considering the mass of solid material (stainless steel) contained in it. The calculation is performed by multiplying the density of the stainless steel ($\rho_w = 7900 \text{ kg/m}^3$) by the volume of the material $V_w$, which depends on the evaporator geometry:

$$M_w = \rho_w V_w$$  \hspace{1cm} (3)

The volume of material is defined as the sum of the volume occupied by the tube fins and the volume occupied by the tube itself:

$$V_w = \left\{ \pi \left[ \left( \frac{d + 2f_{\text{height}}}{4} \right)^2 - d^2 \right] \frac{l}{f_{\text{pitch}}} + \pi \frac{d^2 - (d - 2t)^2}{4} \right\} n_{\text{tubes}}$$  \hspace{1cm} (4)

where $d$ is the tube outer diameter, $f_{\text{height}}$ is the fin height, $s$ is the fin thickness, $f_{\text{pitch}}$ is the distance between consecutive fins along the tube axis, $l$ is the tube length, $t$ is the tube thickness and $n_{\text{tubes}}$ is the total number of tubes. The geometry of the evaporator is explained more in detail in section 2.3.

Fig. 3 illustrates the main steps of the optimization routine. Given the waste heat profile and a suitable working fluid, the first five decision variables are used to design thermodynamically the ORC, i.e. to define the temperatures, pressures and mass flow rates of the cycle. Once the thermodynamic design is known, the evaporator can be designed, so that the number of tubes, heat transfer area and mass of this component can be determined. The ORC thermodynamic and evaporator design data are used as parameters for the dynamic model of the ORC system. The next step involves the tuning of the controllers. For this purpose, the dynamic model of the ORC unit is linearized at design point. After the controller tuning, the dynamic behaviour of the ORC system subjected to the transient heat source profile is simulated. From the simulation, the average net power output of the ORC unit is determined and, together with the evaporator mass, the two objective functions are known. The routine discards all designs that cannot ensure i) a positive degree of superheating, ii) a backpressure of the internal combustion engine below the upper limit or iii) an outlet temperature of the exhaust gas above the lower limit. Details on each single optimization step and on the constraints used for the global optimization are provided in the next subsections.

3.1. Thermodynamic organic Rankine cycle design

The thermodynamic design routine is implemented in MATLAB®. This routine is essential for the subsequent component design, controller tuning and dynamic simulation steps. The main assumptions are as follows: i) all components are considered at steady-state and thermodynamic equilibrium; ii) heat and pressure losses in all components are neglected; iii) the exhaust gas is considered as pure air at 1 bar and iv) the working fluid properties are retrieved from the REFPROP database [38]. The isentropic
efficiencies of the pump, as well as the mechanical and electrical efficiency of the pump motor and inverter are summarized in Table 3. It is important to mention that the appropriate choice of type of expander for mini ORC systems is still an open topic [39,40]. Volumetric expanders are often suggested because of their robustness against possible liquid droplets along the expansion process and low rotational speed [41], but turbines (radial-inflow [42,43], radial-outflow [44] or axial-flow type) can achieve higher isentropic efficiencies and a lower weight-to-power ratio [45]. Several references focused on axial-flow turbines [46–48], including the development of prototypes [45,49] and commercial products [50]. Because of the potential for high efficiency, the expander is assumed here to be an axial-flow turbine. The turbine isentropic efficiency is estimated using the correlations proposed by Macchi and Astolfi [51], which allow including the impact of the working fluid and of the thermodynamic design on the isentropic efficiency of the turbine. In this way, unfeasible or inefficient expander designs can be discarded already in this phase. The isentropic efficiency is a function of the isentropic volumetric ratio, turbine size parameter and the number of turbine stages. The selection of the number of turbine stages is based on the work from Martelli et al. [52], which set a maximum change in specific enthalpy for single stage to 130 kJ/kg and maximum actual volumetric ratio to 15. If one of these constraints is exceeded, the stage is considered not feasible. The number of stages is increased by one, until the conditions are satisfied. The mechanical and electric losses of the turbine and the generator are also summarized in Table 3.

In the thermodynamic design routine, the ORC evaporator is modelled as three subsequent zones depending on the working fluid phase. The routine monitors the temperatures of the exhaust gas and working fluid at the inlet and outlet of each zone to avoid temperature crossings. The condenser is assumed to operate at a fixed condensation temperature of 50 °C. For some working fluids, however, this condensation temperature corresponds to a condensation pressure below the atmospheric pressure. This case has the drawback of requiring a vacuum system to avoid air infiltration, resulting in larger mass, volume and cost of the ORC system. For this reason, two cases are considered, one with and one without the constraint of minimum condensation pressure equal to 1 bar. If this constraint is active, the minimum condensation temperature is equal to the saturation temperature corresponding to 1 bar. It is important to mention that the condensation temperature should theoretically be added to the set of decision variables in Table 2, as done for instance in Ref. [15]. However, since the optimal cooling system design for ORC systems onboard trucks is still an open topic, and given the additional complexity that such considerations would include, the authors decided to leave such considerations as part of future work. More information about the equations used by the thermodynamic design routine can be found in section A of the supplementary material.

### Table 3

| Quantity                                   | Symbol | Value | Unit |
|--------------------------------------------|--------|-------|------|
| Isentropic efficiency of pump              | $\eta_p$ | 70    | %    |
| Combined pump, motor and inverter mechanical and electrical efficiency | $\eta_{PME}$ | 70    | %    |
| Isentropic efficiency of turbine           | $\eta_T$ | according to Ref. [51] | %    |
| Combined turbine and generator mechanical and electrical efficiency | $\eta_{TC}$ | 82    | %    |

3.2. Evaporator design

The evaporator design code is also developed in MATLAB®. Here, the heat transfer area and the mass of the heat exchanger are determined, together with the heat transfer coefficients of the exhaust gas and the working fluid. The dynamic model presented in the next subsection will use this information. The evaporator design routine was originally developed and presented in Pili et al. [19]. The exhaust gas flows in cross-counterflow on the shell-side of a fin-and-tube heat exchanger, whereas the working fluid flows inside the tubes (see Fig. 4). The evaporator is a once-through heat exchanger where the preheating, vaporization and superheating zones are considered as three consecutive lumped zones across the heat exchanger. The evaporator design routine determines the required amount of tubes corresponding to the design heat transfer rate. For the optimization, five decision variables are used, i.e. the fin height, tube outer diameter, fin pitch, tube length and tube.

Fig. 4. Geometry of fin-and-tube evaporator, adapted from Pili et al. [19]: a) tube cross-sectional view, b) tube axial view and c) heat exchanger arrangement.
Spacing. Further details on the modelling and heat transfer correlations used in the evaporator design code are given in Pili et al. [19]. Differently from that work, the tubes are considered here in staggered arrangement in order to enhance the heat transfer. In addition, after a sensitivity analysis, the fin thickness was fixed to 0.5 mm instead of being considered a decision variable of the optimization.

The evaporator causes a rise in the engine backpressure, which penalizes the engine performance in terms of fuel consumption and power. Therefore, this value needs to be minimized. Based on advice from a truck manufacturer, the maximum allowed pressure drop on the exhaust gas side was set to 30 mbar. This value is expected to decrease the engine power output by less than 1% [53]. The pressure drop of the working fluid was set not to exceed 5% of the design evaporation pressure in order not to penalize the net power output of the ORC system. More information about the equations used by the evaporator design routine can be found in section B of the supplementary material.

### 3.3. Dynamic model and simulation

In order to ensure safe and efficient operation of the ORC unit subjected to the highly-transient waste heat profile, a dynamic model is included in the optimization. The model is developed in Simulink® [54]. The dynamic model mainly focuses on the ORC evaporator, which is the link between the heat source and the ORC unit. A moving boundary approach is used, because it provides a reasonable trade-off between model accuracy and computational speed. In the moving boundary approach, the evaporator is divided into three regions depending on the working fluid phase. During operation, the interfaces among the regions can shift, depending on the heat transfer rate. The equations that define the moving boundary model are described in detail in section C of the supplementary material. The inputs to the model are the exhaust mass flow rate and temperature profiles shown in Fig. 1, the maximum allowable pressure [corresponding to 90% of the working fluid critical pressure at off-design] and the design degree of superheating. The latter two are the set points provided to the bypass valve VO controller and the pump mass flow rate 

\[
\dot{m}_{\text{pwf}, P}\ 	ext{controller},
\]

respectively. In the simulation, the variable-step solver 'ode23tb' is used, with a relative tolerance of 2e-3. The condensation pressure as well as the pump inlet temperature of the working fluid are fixed at the design value for simplicity. The model and its verification are described in Ref. [34]. The deviations in terms of degree of superheating from the moving boundary evaporator model available in the TIL library [55] in Dymola [56] based on a 20% step change in working fluid mass flow rate were below 2%. To allow for high computational speed, the heat transfer coefficients \( \alpha \) of both the exhaust gas and the working fluid at off-design ('OD') are corrected from the design values ('D') according to the mass flow rate \( \dot{m} \):

\[
\alpha_{\text{OD}} = \alpha_{\text{D}} \left( \frac{\dot{m}_{\text{od}}}{\dot{m}_{\text{p}}} \right)^\tau
\]  

where \( \tau \) is an exponent derived from fitting and reported in Table 4.

### Table 4

| Heat exchanger side | Region   | Symbol | Exponent \( \tau \) | Unit |
|---------------------|----------|--------|---------------------|------|
| Tube side           | Liquid   | \( \dot{m}_{\text{w}, L} \) | 0.92    | –    |
|                     | Two-phase| \( \dot{m}_{\text{w}, TV} \) | 0.67    | –    |
|                     | Vapour   | \( \dot{m}_{\text{w}, V} \) | 0.86    | –    |
| Shell side          | All      | \( \dot{m}_{\text{es}} \) | 0.54    | –    |

Particular attention is paid to the pressure drop of the exhaust gas \( \Delta p_{\text{eg}} \), because of the negative effect of the engine backpressure on its performance. At off-design, the design exhaust pressure drop is corrected as a function of the square of the exhaust mass flow rate through the evaporator [57]:

\[
\Delta p_{\text{eg, OD}} = \Delta p_{\text{eg, D}} \left( \frac{\dot{m}_{\text{eg, EVA, OD}}}{\dot{m}_{\text{eg, EVA, D}}} \right)^2
\]  

The ORC pump and turbine are modelled at steady-state, since their dynamic responses are much faster than that of the evaporator. While the isentropic efficiency of the pump is kept constant at the design value because of its limited impact on the net power output of the ORC unit, the isentropic efficiency of the turbine is corrected as a function of the mass flow rate according to a correlation presented in Vetter [58]. In addition, while the pump speed is manipulated by the proportional-integral controller, the speed of the expander is assumed to stay constant, because of the lack of suitable correlations to estimate the part-load efficiency of the turbine at variable speed. It is worth mentioning that the constant-speed operation, although less complex, leads to a lower part-load efficiency of the expander with respect to the case where the rotational speed is optimized as a function of the operating point. Given the low speed of sound of organic fluids, it is reasonable to assume sonic conditions to be reached at the turbine nozzle. Therefore, the turbine inlet thermodynamic quantities are related to the mass flow rate at off-design by using the Stodola equation corrected for real gases [59]:

\[
\dot{m}_{\text{w}, T} = \frac{P_{\text{w}, T, in}}{\sqrt{\gamma_{\text{w}, T, in} Z_{\text{w}, T, in} T_{\text{w}, T, in}}} \ 	ext{Kt}
\]  

where \( \dot{m}_{\text{w}} \) is the mass flow rate of the working fluid, \( P_{\text{w}, T, in} \) the pressure, \( \gamma_{\text{w}, T, in} \) the ratio of the specific heats, \( Z_{\text{w}, T, in} \) the compressibility factor and \( T_{\text{w}, T, in} \) the temperature at turbine inlet.

Similarly to the thermodynamic design, the condensation temperature and pressure is fixed at 50 °C or at the condensation temperature corresponding to 1 bar, if the constraint on minimum pressure is applied.

### 3.4. Controller tuning

Two controllers are used to operate the ORC system in a safe and efficient manner: i) one proportional-integral controller manipulates the mass flow rate of the pump \( \dot{m}_{\text{w}, P} \) to achieve the desired set point in terms of degree of superheating at turbine inlet and ii) one proportional controller manipulates the opening of the exhaust gas bypass valve VO when the evaporation pressure exceeds 90% of the critical pressure.

The first controller has the task of ensuring that the turbine always operates with positive degree of superheating, thus avoiding damage and erosion of the turbine blades due to liquid droplets. The set point in degree of superheating could be optimized online or offline, depending on the waste heat mass flow rate and temperature. However, given the rapid fluctuations of the waste heat, a rapid change in set point at low degree of superheating can cause undershoots, and potentially lead to liquid droplets reaching the turbine. For this reason, the set point in degree of superheating is kept constant at the design value, and a constraint in the dynamic simulation excludes designs that cannot satisfy a positive degree of superheating over the driving cycle. By acting on the exhaust bypass valve, the second controller ensures that the system does not work near the critical point, where the working fluid
thermodynamic properties can change considerably and the system can become difficult to control. In addition, if working at higher pressures, the evaporator should be designed to withstand larger mechanical stresses and prevent leakage of the working fluid, resulting in higher costs and mass. The pump and exhaust bypass valve controllers are tuned by linearizing the dynamic model around the design point. After that, the proportional and integral constants of the controller are found by using the standard ‘pid-tune’ command from the Control System Toolbox from MATLAB® [37]. This procedure is repeated at each optimization loop when the dynamic performance is considered.

4. Results and discussion

This section demonstrates the effects of including the dynamic performance in the ORC design procedure, by considering the following two cases: i) a baseline conventional design procedure that neglects the dynamic operation during the design phase, such that the only ORC net power output at design point is maximized and the evaporator mass is minimized with fixed exhaust gas mass flow rate and temperature at the time-weighted values (i.e. 0.223 kg/s and 307 °C) and ii) the novel approach proposed here, where the average ORC net power output considering the dynamic performance (instead of only the design value) of the ORC unit over the profile is maximized and the evaporator mass is minimized. In case ii), the mass flow rate and temperature of the exhaust gas are decision variables and can be changed by the optimizer in each optimization loop across the range of variability reported in Table 2.

4.1. Optimization at time-weighted average conditions of the waste heat source excluding the dynamic performance (baseline method)

In the baseline method, the dynamic performance of the ORC unit is neglected during the optimization phase. Therefore, the algorithm differs from Fig. 3, and is illustrated in Fig. 5. Although the numerical models are the same, it can be seen that the Pareto front is achieved excluding the controller tuning phase and the dynamic simulation from the global optimization loop. Therefore, the objective functions refer only to design conditions (net power output at design point and mass of the evaporator). The average net power output from the dynamic simulation is only calculated after the optimization is completed for a general evaluation of the feasibility and performance of each solution included in the Pareto front.

The multi-objective optimization is carried out for eight working fluids, which previous publications suggested as suitable candidates for waste heat recovery from heavy-duty trucks [17–19,60]. Among them, hydrocarbons, hydrofluorocarbons and hydrofluorochloroolefins are considered. The results of the optimization are shown in Fig. 6. Since the dynamic performance of the system is not investigated here, all parameters correspond to the design point. The optimal solutions result in the Pareto front depicted in Fig. 6a. It is clear that a trade-off exists between the net power output and the evaporator mass. Although it is a complex task to define which exact solutions are feasible to install onboard a truck, it is known that, based on suggestions from a truck manufacturer, the whole ORC system should not exceed 250 kg for a feasible installation. If it is assumed that the share of the evaporator mass is between 30% and 40% of the mass of the entire ORC unit [61], the maximum allowed evaporator mass is between 75 kg and 100 kg. Nonetheless, these values should only be taken as an approximate indication, since it can vary considerably among different truck designs. Given the high level of uncertainty, the Pareto-front solutions shown in the following are not limited to the range 75 kg–100 kg, but can in some situations exceed these values.

The results presented in Fig. 6a indicate that the working fluids that could reach the largest net power output are toluene and ethanol with condensation pressure below ambient (‘LP’ case, which stands for ‘low pressure’), ranging from 3 kW at 23 kg to more than 6 kW at 110 kg. If the constraint of condensation pressure above ambient is imposed, pentane can reach the largest net power output between approximately 3 kW and 4 kW, followed by R1233zd(E), ethanol and R245fa.

Fig. 6b shows that the evaporation pressure is not significantly affected by the Pareto solution. Only for isobutene, there is an increase in evaporation pressure, which ranges from 19 bar to 23 bar. On the contrary, as indicated in Fig. 6c, the degree of superheating shows a large variation along the Pareto front. For all working fluids except ethanol LP, the degree of superheating drops significantly. The degree of superheating is the lowest for toluene, followed by pentane and ethanol, varying between 8 K and 30 K. The trend of the exhaust gas temperature at evaporator outlet is depicted by Fig. 6d. It can be seen that the design outlet exhaust gas temperature drops approximately linearly with increasing ORC net power output. Since the mass flow rate and inlet temperature of the exhaust gas are the same for all designs (they are equal to the time-weighted average of the profile in Fig. 1), there is a larger heat transfer rate in the evaporator for larger ORC net power output. The

Fig. 5. Algorithm of the multi-objective optimization routine at time-weighted average conditions neglecting the dynamic performance during the optimization procedure (baseline case).
maximum heat transfer rate is reached for most working fluids at the minimum heat source temperature at evaporator outlet of 100 °C.

It is important to highlight that the baseline optimization, which excludes the dynamic performance, leads to some of the best Pareto-front solutions having a very low degree of superheating (below 10 K) at design condition. This is in agreement with the results of Ref. [25], where the multi-objective optimization was also based on a fixed heat source close to the time-weighted average. The solutions with low degree of superheating could turn out to be unfeasible, because the fluctuations of the waste heat profile could easily lead to a violation of the constraint of positive degree of superheating during the dynamic operation. Analogously, the exhaust gas outlet temperature is for some optimal designs very close to the lower bound of 100 °C, which will most likely be violated during the driving cycle.

The part-load performance of the ORC unit during the driving cycle presented in Fig. 1 was investigated by carrying out a dynamic simulation for each of the Pareto-front design solutions. Some of the solutions did not converge during the dynamic simulation because of numerical issues related to the infeasible operating conditions and were, therefore, discarded. Fig. 7 shows the time-weighted average of the net power output over the profile for the optimal Pareto-front solutions. Compared with Fig. 6a, it can be seen that the time-weighted average net power output over the profile is lower than the net power output at design, because of the performance degradation of the ORC unit at off-design.
Nonetheless, the results indicate that toluene LP and ethanol LP still achieve the highest power output, ranging from 3 kW at 23 kg to approximately 5 kW in the range between 90 kg and 110 kg. If the constraint of condensation pressure above ambient is imposed, pentane still reaches the highest average net power output at lowest evaporator mass, although a similar average net power output is achieved by ethanol at a much higher mass (115 kg). Furthermore, it is important to highlight that none of the solutions satisfy simultaneously the constraints of positive degree of superheating and exhaust gas outlet temperature above the lower bound during the driving profile. For this reason, no Pareto-front solution resulting from the multi-objective optimization excluding the dynamic performance can be considered technically feasible.

An example of constraint violation due to the dynamic behaviour of the ORC unit over the waste heat profile in Fig. 1 is shown in Fig. 8, for the case of toluene with no limitation on the condensation pressure (toluene LP). For simplicity, only the dynamic behaviour of two Pareto-front optimal points is shown, which are representative of a low mass system (‘LM’, 40 kg of evaporator mass, corresponding to 4.6 kW of net power output at design) and a
high mass system (‘HM’, 80 kg of evaporator mass, corresponding to 5.9 kW of net power output at design). It can be seen that in both the LM and HM cases the constraint of the positive degree of superheating is violated for a considerable amount of time (see Fig. 8a). In the LM case, the fluctuations of degree of superheating are more pronounced due to the lower thermal inertia of the system, whereas the HM system violates the constraint of positive superheating for a longer time due to the slower response. Because of the lower thermal inertia of the evaporator for the LM case, the exhaust gas outlet temperature (Fig. 8b) fluctuates over a broader range for the LM case compared with the HM case. This confirms that the lower thermal inertia of the heat exchanger is less able to level off the fluctuations in waste heat conditions compared with the HM case. It can also be seen that the average exhaust gas outlet temperature for the LM case is higher than that of the HM case, which suggests that a lower average heat rate is transferred from the exhaust gas to the ORC in the LM case. This is because a higher heat transfer rate requires a larger heat transfer area of the heat exchanger, and therefore a larger mass. The dynamic trend of the heat rate is plotted in Fig. 8c, where the dampening effect of the evaporator mass can be seen. In fact, the heat rate from the exhaust gas fluctuates over a very large range (from 10 kW to 85 kW), whereas the heat transfer rate to the ORC working fluid fluctuates between 22 kW and 58 kW (roughly 50% of the oscillation amplitude of the heat rate from the exhaust gas is transferred to the ORC working fluid). Moreover, the results suggest that the minimum heat rate from the exhaust gas is similar for the LM and the HM case, however the maximum exhaust gas heat transfer rate is much larger for the HM case, because of the lower exhaust gas outlet temperature reached by the HM case.

The higher average heat rate from the exhaust gas results in a higher mass flow rate of the working fluid and thus in a larger net power output for the HM case, as shown in Fig. 8d and e. For this reason, the LM case reaches a lower average net power output at off-design compared with the HM case, as previously shown in the Pareto front of Fig. 7 (3.7 kW vs 4.8 kW).

4.2. Optimization including the dynamic performance (proposed method)

As seen in the previous section, excluding the dynamic performance in the optimization loop can lead to constraint violation and unfeasible designs. This section highlights the potential of including the dynamic performance of the ORC unit in the multi-objective optimization, considering only the best working fluids from the multi-objective optimization excluding the off-design dynamic performance carried out in section 4.1: toluene LP, ethanol LP and pentane. The multiple objectives are the ORC net power output and the evaporator mass as in the previous case, but the net power output refers now to the time-weighted average value at off-design from the dynamic simulation instead of only the design value:

$$P_{\text{net, avg, OD}} = \frac{1}{t_f} \int_0^{t_f} P_{\text{net}}(\tau) d\tau$$

(8)

where $t_f = 45$ min is the total duration of the waste heat profile in Fig. 1.

The results of the optimization following the algorithm in Fig. 3 are presented in Fig. 9. The results in Fig. 9a indicate that the Pareto fronts have similar trends as those presented in Fig. 6a, but the absolute values are shifted downwards by approximately 1 kW in net power output. This is because the off-design net power output is used as objective function instead of the design value. Analogously to Fig. 6a, toluene LP reaches the highest net power output, followed by ethanol LP and pentane. Differently from the baseline optimization, the design mass flow rate and inlet temperature of the exhaust gas are not fixed but they are decision variables of the optimization. Nonetheless, it is interesting to see in Fig. 7b and c that both the design mass flow rate and inlet temperature of the exhaust gas are very close to the time-weighted average value used for the baseline optimization, suggesting that is reasonable to use the time-weighted average values for the design of the ORC unit. The maximum deviations of the design exhaust mass flow rate and temperature from the time-weighted average values are found for ethanol LP at an average net power output over the profile below 3 kW, reaching approximately 0.12 kg/s and 35 K. The design inlet temperature of the exhaust gas has a slight increasing trend with rising average net power output for all working fluids, with a deviation between −40 K and 20 K from the time-weighted average. The trend of the design evaporation pressure is shown in Fig. 9d. The results suggest that this quantity remains approximately constant with increasing ORC net power output, analogously to the results shown in Fig. 6c. On the contrary, the design degree of superheating is much larger than for the baseline optimization, with values above 35 K for all working fluids. The degree of superheating drops for pentane and toluene with increasing net power output, whereas ethanol LP shows an increase in degree of superheating at design with increasing ORC net power output, analogously to the baseline optimization case. The design exhaust gas temperature at evaporator outlet is shown in Fig. 9f. The results indicate that analogously to Fig. 6d, the exhaust gas outlet temperature drops with increasing net power output, although ethanol LP has some oscillations below 3 kW. The lower exhaust gas temperature at the evaporator outlet corresponds to a larger heat transfer rate at design, and therefore larger net power output of the ORC unit. For all working fluids the margin of the exhaust gas temperature at the evaporator outlet to the lower bound of 100 °C is larger than those of the baseline case, being above 5 K for Pareto-front optimal solutions.

Similarly to Fig. 8, the dynamic performance of a low mass (‘LM’, 40 kg of evaporator mass, corresponding to 3.0 kW of net power output at off-design) and high mass (‘HM’, 80 kg of evaporator mass, corresponding to 4.2 kW of net power output at off-design) ORC unit is analyzed in Fig. 10 for the proposed optimization method. Given its good performance, the case toluene LP is taken again. The results presented in Fig. 10a suggest that the optimal designs with the proposed method are able to keep the degree of superheating positive over the entire waste heat profile, avoiding erosion of the turbine blades. The HM system has a slower response because of its higher thermal inertia, which leads to higher maximum and minimum degree of superheating over the profile, with the lowest degree of superheating at 5.8 K at 42 min. The exhaust gas outlet temperature is illustrated in Fig. 10b and it can be seen that the oscillations are much larger for the LM case compared with the HM case, due to the lower thermal inertia of the evaporator. The higher evaporator mass of the HM case leads to oscillations of lower amplitude in exhaust gas temperature, and therefore it is possible to design the system for a lower exhaust gas outlet temperature, resulting in a higher average heat transfer rate from the exhaust gas to the evaporator. In other words, a larger heat exchanger allows to smooth better the fluctuations in waste heat, and reduces the risk of acidic condensation of the exhaust gas in the evaporator. In this way, a lower minimum exhaust
gas temperature can be taken to design the ORC unit. This implies that a larger heat rate can be transferred to the ORC unit, and therefore a larger net power output can be achieved, although at the expenses of a heavier system. Fig. 10c shows the trend of the heat transfer rate. The results indicate that the HM mass has comparable minimum but higher peaks in heat rate from the exhaust, resulting in a higher average heat transfer rate from the exhaust gas. It can also clearly be seen that the average heat transfer rate to the working fluid is higher for the HM system compared with the LM system. A higher mass flow rate and a higher net power output are associated with the higher heat transfer rate of the HM case, as shown in Fig. 10d and e.
Compared with the baseline optimization method, it can be seen that the net power output of both the LM and HM cases has much lower amplitude of the oscillations, which can be more favourable for an effective energy management of the vehicle or for a reduction of the system costs because of the lower peaks in maximum power. In fact, the peak of the oscillations in net power output with the proposed method is 67% for the LM case and 74% for the HM case compared to the baseline optimization method. To summarize, the results presented in Figs. 5 and 9 indicate that including the dynamic performance results in higher degrees of superheating and exhaust gas temperatures at evaporator outlet at design condition to avoid the violation of the constraints in terms of superheating degree and exhaust gas temperature at evaporator outlet, ensuring safe operation and avoiding damaging components of the ORC unit.

The optimization with the proposed method including the dynamic performance results in a Pareto-front of feasible solutions since the degree of superheating is always positive and the temperature of the exhaust gas is above the allowed minimum of 100 °C. In addition, the Pareto-front is such that the average net

Fig. 10. Dynamic performance of a low mass (‘LM’) and a high mass (‘HM’) ORC unit designed using multi-objective optimization including the dynamic performance: (a) degree of superheating, (b) exhaust outlet temperature, (c) heat transfer rate, (d) ORC mass flow rate and (e) net power output.
power output of the organic Rankine cycle unit increases as the evaporator mass increases. This means that the evaporator mass that can be transported is the major constraint on the net power output that can be reached. Taking as upper limit 100 kg of evaporator mass as discussed in section 4.1, the best solution in terms of net power output uses toluene with no constraint on the condensation pressure. The average net power output over the waste heat profile for an evaporator mass of 100 kg is 4.5 kW. The optimal decision variables of the optimal design are reported in Table 5.

5. Conclusions

This work presented a novel integrated multi-objective optimization approach for the design of organic Rankine cycle power systems recovering the waste heat from a heavy-duty truck. Two objectives were selected for the optimization routine, i.e. the maximization of the unit net power output and the minimization of the evaporator mass. Unlike a conventional design optimization that excludes the dynamic performance, the multi-objective optimization proposed in this work includes the dynamic performance of the organic Rankine cycle unit in the optimization routine, thus accounting for the performance degradation of the system at off-design and ensuring safe operation also when the system dynamics play an important role. A comparison with a conventional multi-objective optimization based on the time-weighted average values of the heat source mass flow rate and temperature and excluding the dynamic performance was provided.

As for the conventional design, the results suggest that there is a trade-off between the maximum net power output and the minimum evaporator mass, corresponding to a Pareto front of optimal solutions. In addition, the design evaporation pressure does not vary significantly along the Pareto-front solutions, whereas the degree of superheating and the exhaust gas temperature at evaporator outlet vary over a broad range, reaching their minimum at high values of net power output and evaporator mass for most of the working fluids. When the dynamic performance of the organic Rankine cycle unit is included, the degree of superheating and the exhaust gas temperature at evaporator outlet increase considerably for most of the working fluids (more than 35 K and 5 K, respectively), because the waste heat fluctuations during the driving profile require larger margins to satisfy the constraints of positive degree of superheating and exhaust gas temperature above the acidic dew point. The results indicate that both for the conventional optimization and when the dynamic performance is included, toluene achieves the highest net power output for the same evaporator mass, followed by ethanol. However, if the condensation pressure is constrained to be above ambient to avoid the installation of a vacuum system, pentane results in the highest net power output.

The multi-objective optimization routine presented in this work highlights the importance of including the dynamic performance already in the design optimization phase in order to avoid unfeasible or suboptimal solutions. This work provides a methodology through which the optimal working fluid and the optimal set of decision variables can be found, even for a challenging problem as the waste heat recovery from the highly-transient exhaust gas profile of heavy-duty trucks.

CRedIt Author Statement

**R. Pili:** Conceptualization; Data curation; Formal analysis; Funding acquisition; Investigation; Methodology; Project administration; Resources; Software; Supervision; Validation; Visualization; Roles/Writing – original draft; Writing – review & editing. **S. Bojer Jørgensen:** Conceptualization; Data curation; Formal analysis; Conceptualization; Methodology; Validation; Visualization; Writing – review & editing. **F. Haglind:** Conceptualization; Methodology; Supervision; Project administration; Funding acquisition; Visualization; Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

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