

Control Studies of Organic Rankine Cycles with Different Working Fluid Mixtures

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Organic Rankine cycles operate under continuously changing conditions due to enthalpy variations in the hot source, uncertainty in the thermodynamic properties of novel working fluid mixtures, variable efficiency in the expander and the heat exchanger units, and malfunctions in the pumping system. An optimal model based control system can effectively alleviate the influence of exogenous disturbances and uncertainty from the changes in the operating specifications. The performance of such a controller applied on an ORC system that uses as a working fluid a mixture of two components is investigated in the present work. Multi-component mixtures as working fluids in ORC systems can substantially improve the overall efficiency and reduce the exergy losses due to better proximity between the hot source and the working mixture temperature profiles compared to a system with a pure component as the working medium. Previously identified as potentially good working fluids in terms of thermal and exergy efficiency under steady state conditions are being investigated for their dynamic performance under closed loop conditions. The study provides an additional criterion for the ultimate selection of the most suitable working fluid candidate.

1. Introduction

Recently, organic Rankine cycle (ORC) systems have attracted significant attention due to their ability in recovering low-grade heat through a process flowsheet of low complexity and relatively straightforward in terms of maintenance. The increasing popularity of ORC is also justified by the ability of the cycle to adjust in order to accommodate the utilization of heat from various energy sources. ORC applications employ among others solar, geothermal, biomass, and combustion based hot sources. Most of these energy sources have an intermittent nature, which implies that the available heat load may vary with time quite significantly. On the other side, the ORC system must provide a relatively steady power load as required by either grid regulations or the application characteristics. In addition, the variable conditions at the hot source side of the system may affect the mechanical integrity of the ORC components and therefore specific temperature and pressure limits are imposed within the cycle. For instance, two phase flow in the expander could severely compromise the integrity of the expander due to erosion and increased mechanical strain. Transient phenomena may cause significant deviations from the acceptable range of operating conditions causing the deterioration of the achieved cycle performance. The solution relies on the installation of an appropriate control system that is able to maintain optimal operation without undesirable fluctuations despite the influence of exogenous disturbances and the presence of uncertainty. The control system if tuned properly will successfully transfer variability from key and performance sensitive variables to less important in terms of energy efficiency and economics variables.

Recently published literature has recognized the need to thorough study the dynamics of ORC systems and indicated the necessity for the development efficient control strategies (Linke et al., 2014). Lee et al. (2012) studied the transient response of a 50 kW ORC system utilizing R-245fa as the working medium, subject to variations in the secondary fluid flow rate in the condenser that affects the generated electric power. Pierobon et al. (2014) proposed the integration of transient performance analysis into the ORC design procedure. A preliminary assessment of system configurations was employed in order to enhance dynamic performance for a pre-specified working medium. Casella et al. (2013) studied a 150 kW high-temperature turbo-generator and

developed a methodology in order to examine the dynamic response of an ORC power system using toluene as the working fluid of the process.

Hou et al. (2014) studied an online self-tuning generalized minimum variance controller for a given working medium. Zhang et al. (2014) proposed a model predictive control system for controlling a waste heat conversion system. The analysis focused on the control of the evaporator pressure, the superheating temperature and the condenser outlet temperature. Quoilin et al. (2011) studied the dynamic performance and the control of an ORC waste heat recovery system with R-245fa as the working fluid. They proposed three different control strategies and recommended the most successful by considering the optimised evaporating temperature based on the prevailing operating conditions. Jolevski et al. (2017) proposed a decentralized control structure by loop pairing using the non-square relative gain array and dynamic non-square relative gain array methods.

Currently, the selection of working fluid mixtures is based on thermodynamic performance indicators at steady-state conditions (Mavrou et al., 2014) but does not consider at all the dynamic behavior of the ORC system under the presence of disturbances. A designed controller with the proper tuning, counteracts the influences of exogenous changes and contributes to the optimum economic performance of ORC system. However, the response of the control system greatly depends on the sensitivity of the working fluid properties to the operating conditions. Disturbances may cause deviations from the design point and therefore working fluids that exhibit low sensitivity in their properties when operating conditions change would react more steadily on the commands from the control system. On the contrary, highly sensitive working fluids will not support the control system towards the alleviation of the disturbance effects. Mavrou et al. (2015) observed that the preliminary selection of working fluids and ORC operating characteristics, which present minimum sensitivity to variability is important for the economic performance of the ORC system as operating conditions drifted away from those at the nominal design point. Recently, Papadopoulos et al. (2017) generalized the approach by proposing a systematic methodology that concerns the integration of variability within the Computer-Aided Molecular and Process Design (CAMPD). The static operability analysis that was proposed seemed to approach the realistic problem representation, however process dynamics were not considered explicitly. This work aims to further expand these two works in the field of ORC systems through the incorporation of direct dynamic simulation for an optimal control system.

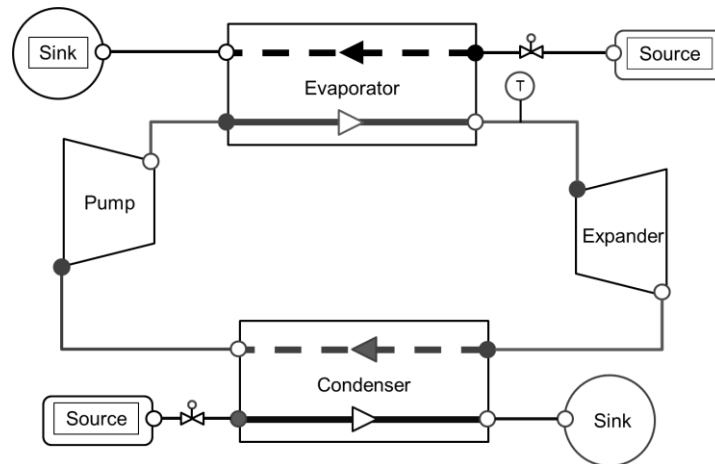


Figure 1: Conceptual flowsheet of an ORC model.

2. Proposed developments

2.1 Main considerations

It is remarkable to observe in all previously published works that control studies in ORC systems involve exclusively working fluids consisted of pure substances. This study aims to investigate the impact of mixtures in transient performance, since they improve ORC efficiency in steady-state models (Papadopoulos et al., 2013). The reason for such improvement is the drastic reduction of exergy losses due to the closer distance between the hot source and the evaporating mixture temperature profiles in the evaporator compared to a system with a pure component as the working medium.

To this end, a dynamic model of the cyclic process was developed. An ORC system is usually consisted of two heat exchanger units, namely an evaporator and a condenser, an expander and a pump as it is shown in Figure 1. For each working fluid mixture considered the optimal sizing of the ORC system equipment and the optimal operating conditions are calculated that maximize the achieved overall thermal efficiency of the system. This is performed through nonlinear mathematical programming techniques that utilize a steady-state model for the

ORC system along with suitable constraints that guarantee a safe operation. In this way, each working fluid mixture would be able to perform in the most efficient way and therefore the basis for comparison is facilitated. In addition, for each optimal ORC design for the given working fluid mixture, a control system is developed that aims to maintain the operating performance near the optimal point despite the influence of disturbances affecting the system. Instead of using multiple control loops a centralized control algorithm is preferred. An optimal model predictive control algorithm is employed that uses a dynamic model of the ORC system to predict the impact of the control actions to the dynamic response of the system. A control performance index expressed in terms of deviations from the desired thermal efficiency for the system that also penalizes the rate of change for the manipulated actions is defined. The control actions that optimise this control performance index are then calculated.

Such a control algorithm would take explicitly under consideration the interactions among the various subsystems (e.g., evaporator, expander and so forth) in the cyclic system. The influence of the working fluid on the control system dynamic performance can then be evaluated by comparing the thermal efficiency behaviour in closed loop conditions under the presence of disturbance. This present study evaluates and rank-orders some of the most promising working mixtures identified by Papadopoulos et al. (2013) using a computer aided molecular and process design (CAMPD) approach. Dynamic control system performance becomes an additional factor in determining the most suitable working medium for the given ORC system.

2.2 Evaporator and Condenser model

The proposed dynamic model integrates the dynamic energy balances accompanied by constitutive equations for the evaluation of the thermodynamic properties. It also involves a number of empirically defined relations for the estimation of the heat transfer coefficients, as well as the efficiencies for the expander and the pump. The dynamic model of the evaporator and condenser generates the evaporation and the condensation temperature profiles of the working fluid mixture. Evaporation temperature profile affects the performance of the ORC and should be kept within a specific range in order to achieve higher energy efficiency and guarantee safe operation. A constant pressure drop along the length of the reaction is specified. The heat exchanger is spatially discretised according to the finite volume method. Eq(1) describes the energy balance in each heat exchanger compartment, where $V(\text{m}^3)$ is the volume of the heat exchanger compartment, ρ (mol/m^3) is the density of the working fluid, \dot{M} (mol/s) is the mass flow rate, h_{out} (J/mol) is the output stream enthalpy, h_{in} (J/mol) is the input stream enthalpy and \dot{Q} (J/s) is the heat transferred to the working fluid.

$$V \cdot \rho \cdot \frac{dh}{dt} + \dot{M} \cdot (h_{out} - h_{in}) = \dot{Q} \quad (1)$$

2.3 Expander and pump

The dynamic behaviour of the expander and pump is much faster than the heat exchangers and therefore a pseudo steady-state model was applied to both units. Eq(2) defines the expander overall isentropic effectiveness ε_s which is assumed equal to 0.7 and Eq(3) defines the pump internal isentropic efficiency, ε_{ieff} which is assumed equal to 0.78. W (J/s) is the power produced, $h_{in,exp}$ (J/mol) is the inlet enthalpy, $h_{out,exp,s}$ (J/mol) is the outlet enthalpy in the expander. $h_{out,p}$ (J) and $h_{in,p}$ (J) are the output and inlet enthalpy of the pump. $p_{in,p}$ (Pa) and $p_{out,p}$ (Pa) are the input and output pressures in the pump, and $v_{in,p}$ (m^3) is the pump volume.

$$\varepsilon_s = \frac{\dot{W}}{\dot{M}(h_{in,exp} - h_{out,exp,s})} \quad (2)$$

$$\varepsilon_{ieff} = \frac{v_{in,p} \cdot (p_{out,p} - p_{in,p})}{h_{out,p} - h_{in,p}} \quad (3)$$

3. Optimal design and control problem formulation

Eq(4) describes the objective function of the steady-state optimisation problem of the ORC system with nominal capacity equal to 1 kW, for the maximisation of its thermal efficiency. X is the vector of state variables (basically all variables associated with the process units in the ORC system), whereas d is the vector of decision variables as shown in Eq(5). Q_{ev} is the heat provided in the evaporator and W_{exp} is the produced work in the expander, and W_{target} is the specified power capacity of the ORC. A_{evap} and A_{cond} denote the heat exchange area for the evaporator and the condenser, respectively. F_{wf} is the flowrate of the working fluid and FH_2O_{evap} and

FH_2O_{cond} are the inlet flowrates of secondary fluid in evaporator and condenser. The solution of the design optimisation problem is subject to the modeling equations Eq(1)-(3).

$$\min_d J(X, d) = (W_{exp} - W_{target})^2 + Q_{ev} \quad (4)$$

$$d = [A_{evap} \quad A_{cond} \quad F_{wf} \quad FH_2O_{evap} \quad FH_2O_{cond}]^T \quad (5)$$

The steady-state design optimisation problem is solved using a nonlinear programming technique as implemented in MINOS 5.5. (Murtagh and Saunders, 1983).

The control problem aims to maintain the ORC performance near its optimal operating point despite changes in the thermal conditions of the hot stream. A model-based predictive controller calculates a sequence of actions for the manipulated variables in the system that satisfies a performance index (Kyriakides et al., 2016). The performance index for the MPC attempts to keep the evaporator working fluid outlet stream temperature at the desired level, T_{sp} , using as manipulated variables, u , the flow rates of the hot and the cold water streams in the evaporator and the condenser as shown in Eq(6). Constraints in the form of variable bounds are defined for both the manipulated variables and the rate of change for the manipulated variables in order to impose physical and operational limits, Eq(7).

$$\min_{\Delta u} \left(\sum_{i=1}^{N_p} (T_{sp} - T_{evap,out}(k+i))^T Q (T_{sp} - T_{evap,out}(k+i)) + \sum_{i=1}^{N_c} \Delta u(k+i-1)^T R \Delta u(k+i-1) \right) \quad (6)$$

$$\Delta u^{min} \leq \Delta u \leq \Delta u^{max}, \quad u^{min} \leq u(k) \leq u^{max} \quad (7)$$

N_p is the prediction horizon and N_c is the control horizon. Matrix Q of size $(N_p \times N_p)$ determines the importance of each controlled variable along the prediction horizon. Matrix R of size $(N_c \times N_c)$ imposes a penalty on the rate of change for each manipulated variable along the control horizon. The control problem is solved as a quadratic program at each time interval with the control actions parameterised in a piecewise constant fashion. The use of the rate of change for the manipulated variables, Δu , instead of the actual control action, u , in the objective function makes the optimisation problem formulation consistent with the a zero steady-state error behaviour. At each time interval the first control action is implemented and the new state of system is obtained at the end of the time interval. Considering also an integrating error model, the MPC formulation is equipped with integral action that guarantees zero steady state offset.

4. Case study and results

To investigate the impact of mixtures in ORC control performance two different mixtures at eight different concentrations are considered, as shown in Table 1. Mixtures M1 and M2 have been proposed by Papadopoulos et al. (2013) as novel working fluids through a systematic CAMPD approach that exhibit optimum economic performance. Table 2 shows the investigated mixtures and the respective decision variables for the ORC as they are calculated from the steady state optimisation problem of Eq(4).

Table 1: Investigated working fluid mixtures (Papadopoulos et al., 2013)

ID	Investigated concentrations	Component 1	Component 2
M1	30, 40, 60, 70%	1,1,1-Trifluoro-propane [CH ₃ -CH ₂ -CF ₃ /CAS:421-07-8]	2-Fluoromethoxy-propane [FCH ₂ -O-CH-(CH ₃) ₂ /CAS:-]
M2	30, 40, 60, 70%	1,1,1-Trifluoro-propane [CH ₃ -CH ₂ -CF ₃ /CAS:421-07-8]	1-Fluoromethoxy-propane [FCH ₂ -O-(CH ₂) ₂ -CH ₃ /CAS:-]

Novel fluids and especially mixture 30%M1 achieves the best thermal performance in comparison with the other investigated mixtures. It is important to investigate whether such performance can be maintained under the effect of disturbances in closed loop. Based on the optimal design an MPC is developed and tested for its ability to achieve the desired dynamic behaviour. Using a sampling interval of 5 s, the prediction horizon length was selected to be equal to 12 time intervals and the control horizon to be equal to 6 time intervals. Q and R are diagonal matrices with all diagonal elements equal to unity.

Table 2: Decision variable values for each mixture after optimisation.

ID	A_{evap} [m ²]	A_{cond} [m ²]	F_{wf} [mol/s]	$F_{\text{H}_2\text{O}_{\text{evap}}}$ [mol/s]	$F_{\text{H}_2\text{O}_{\text{cond}}}$ [mol/s]	$\eta_{\text{eff}}\%$
30 %M1	1.55	2.68	0.166/0.388	10.00	6.593	5.91
40 %M1	1.94	2.27	0.279/0.418	11.52	12.02	4.79
60 %M1	2.88	2.34	0.446/0.297	6.475	10.75	4.79
70 %M1	2.53	2.12	0.495/0.212	6.101	10.79	5.19
30 %M2	1.91	2.91	0.184/0.430	10.00	7.672	5.08
40 %M2	2.30	2.63	0.275/0.413	8.58	10.56	4.67
60 %M2	3.62	1.61	0.44/0.294	5.66	77.07	4.75
70 %M2	1.54	1.66	0.495/0.212	20.00	25.16	5.15

Figure 2a depicts the percentage change in the work of the expander for a 3.7 °C change in the hot stream temperature (Figure 2b) for the selected working fluids under closed loop conditions. Mixture 60 %M2 and 60%M1 maintain the expander work closer to the given setpoint than the other working fluids. The secondary fluid flow rate in the evaporator, which is one of the two manipulated variables reached its upper bound during the occurrence of the disturbance as shown in Figure 3. The superior performance of some mixtures against the others is mainly due to the sensitivity of their properties with respect to the changing operating conditions. The disturbance drifts the process away from the desired conditions, while the controller attempts to quickly counteract the deviating behaviour. The controller limits the observed variation in the operating conditions despite the saturation in the manipulated variables and therefore the differences in the dynamic performance are not very large. A working fluid with properties that are sensitive to the prevailing conditions would make the effort to compensate the effects of disturbances much larger. This implies that the deviation from the load specification would grow even larger. A less sensitive fluid would maintain its ability to compensate for the disturbance for a wider range of process conditions.

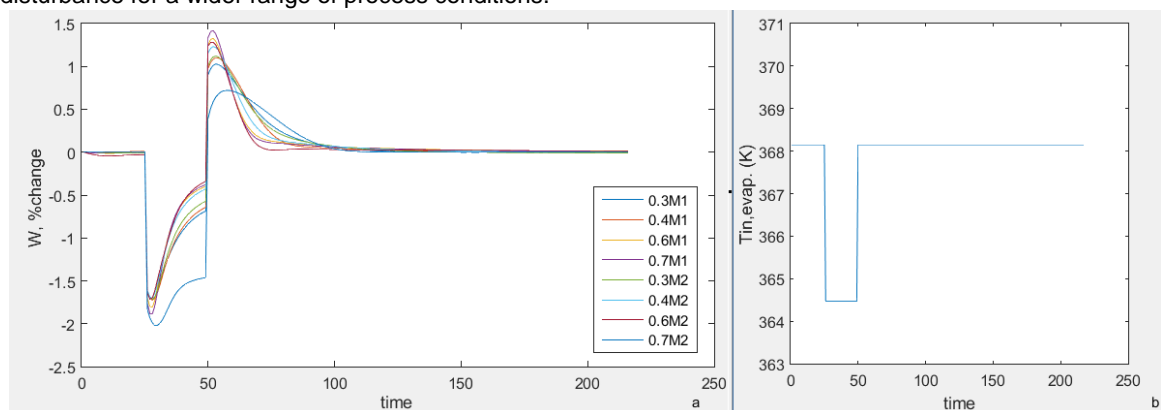


Figure 2. Expander work % change (a) for eight working mixtures and (b) imposed disturbance in the secondary fluid's inlet stream temperature in the evaporator.

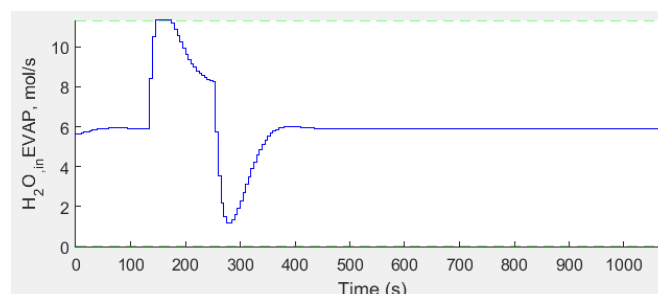


Figure 3. Manipulated variable (u_1) for 60 %M2 of the ORC system.

5. Conclusion

A number of different mixtures acting as working fluids in an ORC system have been evaluated on their ability to perform adequately under closed loop conditions. A model predictive controller with constraints was employed for each optimally designed ORC system with each given working fluid. The dynamic performance for a specific disturbance scenario was calculated and assessed for all working fluids. The differences in the observed dynamic response were mainly attributed to the sensitivity that the working fluid properties have on the operating conditions. Such sensitivity behaviour can be used as an additional criterion in a working fluid selection procedure.

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