Energies **2015**, *8*, 4755-4801; doi:10.3390/en8064755

OPEN ACCESS

energies

ISSN 1996-1073

www.mdpi.com/journal/energies

Review

Systematic Methods for Working Fluid Selection and the Design, Integration and Control of Organic Rankine Cycles—A Review

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Academic Editor: Roberto Capata

Received: 1 March 2015 / Accepted: 15 May 2015 / Published: 26 May 2015

Abstract: Efficient power generation from low to medium grade heat is an important challenge to be addressed to ensure a sustainable energy future. Organic Rankine Cycles (ORCs) constitute an important enabling technology and their research and development has emerged as a very active research field over the past decade. Particular focus areas include working fluid selection and cycle design to achieve efficient heat to power conversions for diverse hot fluid streams associated with geothermal, solar or waste heat sources. Recently, a number of approaches have been developed that address the systematic selection of efficient working fluids as well as the design, integration and control of ORCs. This paper presents a review of emerging approaches with a particular emphasis on computer-aided design methods.

Keywords: organic Rankine cycle; systematic approaches; design; optimisation; working fluid selection

1. Introduction

Over the past decade increasing concerns over climate change and high energy prices have resulted in a strong interest to utilize waste or renewable heat sources for power generation. For such applications the Organic Rankine Cycle (ORC) is a widely used technology with many installations converting a number of heat sources to power in the kW and MW range [1]. The success of the system is largely attributable to its simplicity and flexibility: ORCs are simple Rankine cycles similar to those used in conventional power plants. ORCs are flexible and can be applied on a wide range of heat source temperatures ranging from 80 to 400 °C [2]. They enable cost efficient power generation from a broad range of heat sources by replacing water with organic working fluids such as refrigerants and other organic molecules to achieve better efficiencies [3]. Although ORCs constitute a proven technology with more than 1.5 GW_{el} of capacity installed world-wide in a variety of applications, including industrial waste heat recovery [1], geothermal [4–6], solar thermal [7] and biomass power plants [8], the key research challenges remain: the identification of high-performance working fluids, the corresponding optimal design configuration and operating characteristics of the thermodynamic cycle and the optimum integration of the ORCs with the available heat sources.

The design challenge is due to the very large number of working fluid chemistries as well as structural and operating ORC parameters that need to be considered as decision options within a systematic problem formulation to identify highly performing systems. The examination of various working fluids or alternative ORC configurations can lead to useful insights regarding potential performance improvements, yet most published works lack the use of systematic methods, rather relying on empirically identified enhancements approached through heuristic treatment of decision options. Empirical investigations are often based on knowledge gained from either experimental or theoretical work and are clearly useful. Yet the proposed improvements may be limited unless an extensive number of ORC working fluid and system characteristics are systematically taken into account during optimization.

Computer-aided technology is a promising tool to exploit empirical know-how and guide the search for novel and efficient technologies as it is capable to cope with the investigation of an enormous range of options [9]. Process design and optimization [10], process integration [11], control [12], molecular design [13–15] and integrated process and molecular design [16] are examples of systematic computer-aided methods with applications in diverse process systems.

Research and development efforts in ORC have made use of computer-aided tools and methods in the past, but they have rarely been used in a systematic context. The use of systematic and robust computer-aided methods in the development and operation of ORC technologies has emerged in the last few years, but it is still limited compared to the very widespread application of similar tools in other technological sectors. Considering the benefits reaped from the application of such tools in other industries, there is great scope for widening their utilization in ORC. There is currently a very wide community of engineers and scientists in ORC research and development, who are beginning to grasp the benefits resulting from use of systematic computer-aided tools.

This paper aims at presenting a review of available systematic methods for working fluid selection and the design, integration and control of ORCs. The scope of the paper is focused on subcritical ORCs. It provides a structured and organized account of the merits of selected works for more efficient

technological developments and identifies areas for further research into computer-aided tools and methods for ORC systems engineering.

2. Overview

The basic ORC process for converting heat from a source stream to power consists of a pump, a turbine, a heat source recovery section and a condenser and uses an organic compound as the working fluid. In the heat recovery section, heat is transferred from the hot source stream to generate high pressure working fluid vapor from which power is generated in a turbine. In the condenser, heat is ejected to a cold utility from the low pressure working fluid vapor obtained from the turbine outlet. The resulting liquid working fluid is repressurized in the pump and the cycle is closed in the heat recovery section.

The overall design goal is to maximize ORC system performance for a given situation in terms of heat sources and heat sinks. Different performance criteria have been used as design objectives in ORC studies [17], the most common being the thermodynamic metrics thermal efficiency and exergetic efficiency, with economic criteria such as the power production cost being less common due to the difficulties of precise cost estimation.

The development of a high performance ORC system with respect to any typical performance criterion requires good design choices to be made across the cycle and its interfaces with the heat sources and heat sinks. Important design decisions need to be made with respect to working fluid selection, the cycle design and its operating conditions as well as the heat recovery strategy from the available heat sources, which may involve one or more source streams (Figure 1).

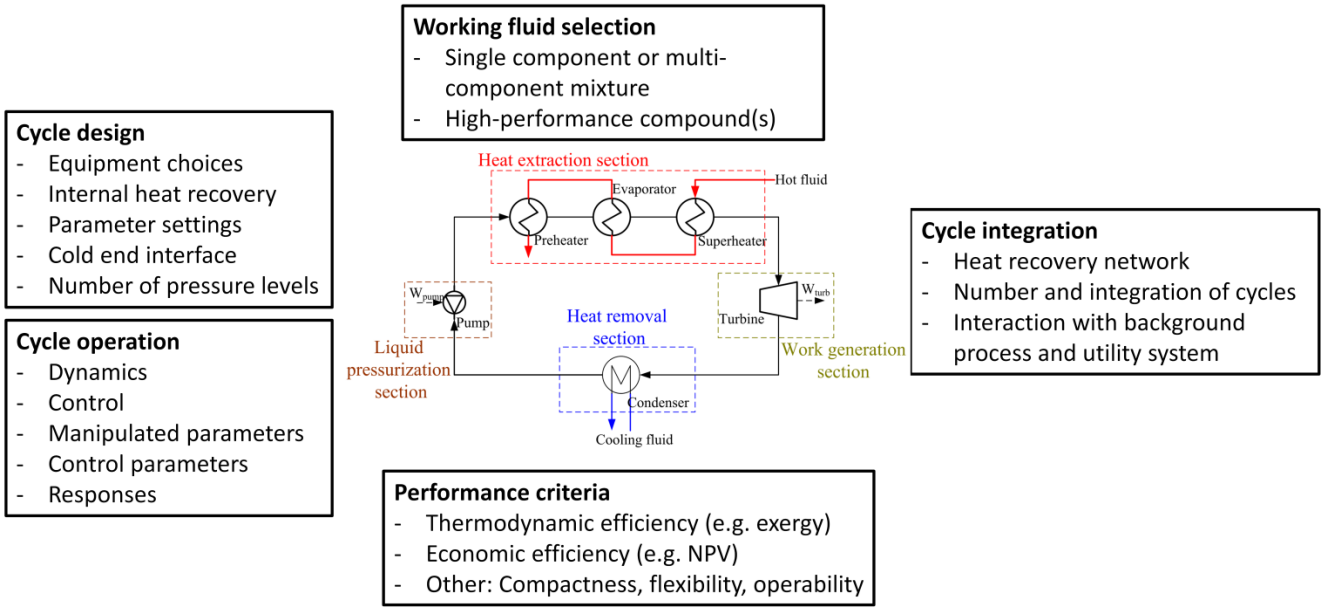

Figure 1. ORC design decisions and objectives.

Many design alternatives exist at each level. For instance, a very large number of alternative working fluids exist, some of which may have never been proposed for ORC systems before. The identification of the best performing working fluid for a given situation requires the ability to systematically screen through the alternatives. Similarly, heat may be transferred from multiple available heat sources so that many alternative strategies may exist to recover the heat into the working fluid. In addition, cycle

operating parameters must be optimized to ensure alternatives are compared on the basis of the best possible performance.

Over the years, a number of systematic approaches have emerged to support the designer in optimizing and analyzing alternatives so as to effectively identify the high performing ORC designs for a given problem. These will be reviewed in the remainder of this paper. Section 3 will review systematic approaches to working fluid selection. Section 4 will provide an overview of cycle optimization approaches before approaches to ORC control are reviewed in Section 5. Emerging approaches to the integration of ORCs with multiple heat sources will be reviewed in Section 6.

3. Design and Selection of ORC Working Fluids

3.1. Working Fluid Selection Applications

The choice of ORC working fluids is known to have a significant impact on the thermodynamic as well as economic performance of the cycle. A suitable ORC fluid must exhibit favorable physical, chemical, environmental, safety and economic properties such as low specific volume, viscosity, toxicity, flammability, ozone depletion potential (ODP), global warming potential (GWP) and cost, as well as favorable process attributes such as high thermal and exergetic efficiency, to name but a few [4,5,17–19]. These requirements apply both to pure and mixed working fluids. Existing research is largely focused on the selection of pure working fluids, with well over 100 published reports currently available (see surveys in [1,20]). An important limitation of pure working fluids is their constant temperature profile during phase change [18]. The pinch point encountered at the evaporator and the condenser gives rise to large temperature differences at one end of the heat exchanger leading to high irreversibility. The pinch point is a point of minimum temperature difference between the heat source and the working fluid side of the heat exchanger where the heat transfer is blocked. Working fluid mixtures are more appealing than pure fluids because their evaporation temperature profile is variable, following the profile of the heat source, as opposed to the flat evaporation profile of pure fluids. This enables an approximately stable temperature difference during evaporation, coined as temperature glide, which significantly reduces exergetic losses. Despite their usefulness, the published works addressing the selection of mixed fluids are considerably fewer. Previously published work [21] has investigated different types of multi-component mixtures comprising hydrocarbons, hydrofluorocarbons or siloxanes together with important mixture performance measures and constraints that need to be considered for their evaluation. Hydrocarbon mixtures were also proposed considering regenerative preheating ORC schemes [22], equipment sizing [23] and zeotropic fluids [24] for efficient exploitation of moderate temperature geothermal resources. Mixtures of siloxanes or hydrocarbons have been considered [25] to recover wasted heat from molten carbonate fuel cells using an ORC. Halocarbon mixtures have been investigated [26] for power generation using geothermal heat, indicating significant ORC performance gains compared to pure fluids. A binary mixture of fluorocarbons has been investigated [27] at different concentrations employed in an ORC system for power generation from solar energy. In a similar context, the utilization of hydrocarbon and fluorocarbon mixtures has been investigated [28] at different temperature heat sources in ORCs, evaluating the resulting performance gains using ORC operating parameters like inlet/outlet volume ratio, mass flow, enthalpy difference of expansion *etc.* Different combinations of binary and tertiary

mixtures have also been evaluated [29] including alkanes, fluorinated alkanes and siloxanes aiming to find their optimum concentration. An investigation of organic, ammonia-water and alcohol-water mixtures was performed using an optimization method to identify their optimum concentration in ORC and Kalina cycle systems [30]. Mixtures of ammonia- water and CO_2- water were also considered in two new ORC configurations, namely the ORC with liquid-flooded expansion and the ORC with solution circuit [31], with the mixtures employed in the second configuration only. An ammonia-water mixture was also considered in the context of a Kalina cycle and its performance was compared with an ORC using pure ammonia or R134 [32]. Nineteen binary working fluid mixtures were also considered as an alternative to ammonia-water, resulting in the conclusion that the highest performers were propane and propylene-based mixtures. Binary and tertiary polysiloxane mixtures are considered in a different work [33] for ORCs recovering heat from cogeneration plants fed with wood residuals. A zeotropic mixture of R227ea/R245fa is analyzed in a subcritical ORC employed for exploitation of geothermal resources [6].

Whether pure or mixed working fluids, conventional engineering practice mostly considers their selection by testing and comparing various known options from a pre-postulated dataset of several available candidates. As a result, the search is limited to an often arbitrarily compiled list of candidates containing conventional molecules (e.g., refrigerants, hydrocarbons *etc.*). Such a small set is extremely limiting in view of the vast number of molecules that could be considered as candidate ORC working fluids, hence significantly reducing the opportunities for identification of novel and improved options. The limited screening of potential working fluid candidates hampers innovation and a systematic approach is required to enable wider and more systematic searches. The latter is very relevant to the necessity for development of novel chemical compounds which may exhibit favorable characteristics as ORC working fluids and may also overcome the performance of existing ones. In conventional practice this is only possible through experimental work which is clearly useful and irreplaceable. However, experiments involve high costs which are often not justified by the limited performance gains. Computer-aided tools may assist experimental work through their predictive capabilities by systematically guiding searches to options worth investigating. The rather ad-hoc use of such tools in conventional practice prohibits such opportunities.

3.2. Computer-aided Tools: Main Concepts and Challenges

The use of computer-aided tools is clearly very appealing for either the design of novel working fluids or the selection of commercially available ones, in both cases with optimum performance characteristics. The term “design” refers to the determination of a molecular structure regardless of whether such a molecule pre-exists or not. The achievement of optimum performance is rather challenging because it involves two major requirements:

a) The exhaustive generation and evaluation of a very wide range of molecular structures prior to the selection of the working fluid which exhibits a truly optimum performance.
b) The utilization of predictive models which are sufficiently accurate to ensure that the performance of the selected working fluid is both optimum and rigorously validated prior to its practical utilization in an ORC plant.

These requirements are conceptually illustrated in Figure 2 with the aim to provide a comparative assessment of the general predictive model types available to simulate molecular chemistry characteristics and the range of molecules that may be evaluated with each model type within a reasonable computational efficiency. The three model types involve computational chemistry methods, equations of state (EoS) and group contribution (GC) methods in a representation that implies a complementarity due to the existence of shared features that reflect common phenomena and functionalities captured by adjacent models of different abstraction (*i.e.*, rigor of the modelling detail). The simultaneous utilization of representatives from all model types would be ideal as it would satisfy both previous requirements for the identification of optimum and immediately applicable working fluids, yet it would have a detrimental effect on computational efficiency. This is also the main reason why each type of model may only be used independently but not all types are suitable for the optimum design and selection of highly performing working fluids.

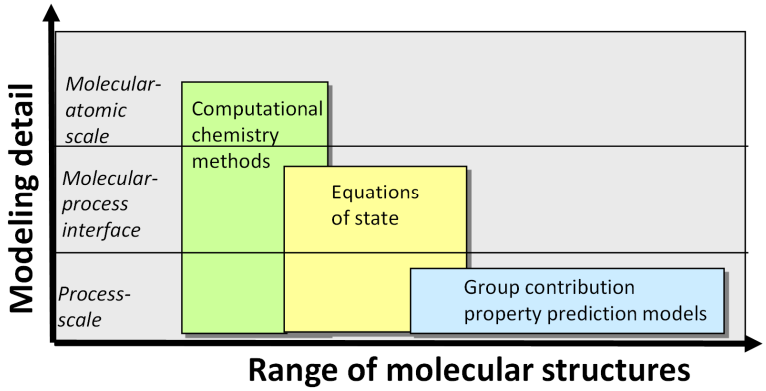

Figure 2. Property prediction models with respect to modeling detail and range of molecular structures which may be simulated at a reasonable computational effort.

Computational chemistry methods [34] involve several different techniques such as density functional theory (DFT) and the conductor-like screening model for real solvents (COSMO-RS) [35] which is based on quantum chemistry and addresses liquid phase predictions. Such methods are based on a robust representation of the molecular chemistry hence they enable the determination of property features at even the atomic or molecular scale. However, the resulting predictions may not be easily transferred into molecular parameters which are required to performed mass and energy balances or to determine operating conditions at the ORC process level. Furthermore, the simulation of even one molecule often requires very extensive computational effort which may range from a few hours to a few days hence prohibiting their use to evaluate the vast number of molecules that may be considered as ORC working fluids. On the other hand, EoS act as an interface between molecular characteristics and process-level properties, while the required computational effort is sufficiently low to use them in an extensive evaluation of working fluids. However, chemical or physical parameters required as inputs to characterize molecular or mixture behaviors are available for relatively few molecules, prohibiting the direct and wide utilization of EoS in the design and selection of working fluids.

GC methods [36] avoid the bottlenecks of computational efficiency and data unavailability because they are based on relatively simpler (hence computationally faster) predictive models than the other two methods, while they refer to molecular fragments called functional groups instead of entire molecules.

This solves the problem of data unavailability because if the contribution of each functional group in a particular property is calculated once, then it remains the same regardless of the molecular structure in which it is used (*i.e.*, it is transferable in different molecules). As a result, simpler or complex molecular properties are calculated using GC models developed around databases of experimentally pre-determined property contributions for each functional group. GC methods provide predictions which are sufficiently accurate so that large molecular sets may be easily screened and few selected molecules of high performance in desired properties may then be validated using EoS, computational chemistry methods or experiments. Despite their obvious advantages they are challenged by the need to pre-specify a molecular structure (e.g., an ORC working fluid) in order to calculate its property values. This characteristic is also shared with EoS and computational chemistry methods and requires some prior knowledge regarding molecular structures that may lead to optimum ORC performance, otherwise the exhaustive examination of every possible molecule that exists is unavoidable in order to ensure the identification of a truly optimum ORC working fluid.

3.3. Optimization-Based CAMD of Pure Fluids

The above challenges are efficiently addressed by computer aided molecular design (CAMD) methods which combine the merits of GC methods with optimization algorithms. Papadopoulos *et al.* [4,5,37] proposed such an approach where an optimum molecule with desired properties is automatically identified based on the computational emulation of a molecular synthesis process (*i.e.*, the iterative transformation and evolution of an initial structure using different combinations of functional groups). An optimization algorithm guides the synthesis towards optimum structures, using properties as performance measures that reflect on molecular or process characteristics. The combination of GC methods with optimization also proves useful when a pre-specified database of molecules exists and requires fast screening to efficiently identify highly-performing options. CAMD approaches cover a very wide range of potentially optimum structures, support the identification of either novel molecular structures or conventional but previously overlooked, optimum molecules and rely on robust and systematic algorithms. Properties may be calculated by simpler GC models capturing the molecular chemistry effects on major ORC operating characteristics. EoS models may also be used (in combination with GC representations or not) to directly link molecular structure with ORC process economic and operating performance. Figure 3 illustrates the algorithmic steps involved in the optimization-based CAMD approach used in Papadopoulos *et al.* [4,5]:

- The selection of several functional groups from a database enables the generation of a molecule that is tested in terms of chemical feasibility.
- The desired properties of any feasible molecule are subsequently calculated based on the contribution of each functional group in the molecule.
- Several of these properties are used as a measure of molecular performance, *i.e.*, as objective functions in the employed optimization algorithm. The employed properties may directly reflect molecular characteristics or ORC process features.
- The optimization is then used to assess the performance based on specific algorithmic criteria and to inflict alterations in the molecular structure using functional groups available in the database, in order to generate a new molecule.

- This iterative procedure continues until a molecule with the optimum performance is identified, based on algorithmic termination criteria that ensure optimality.

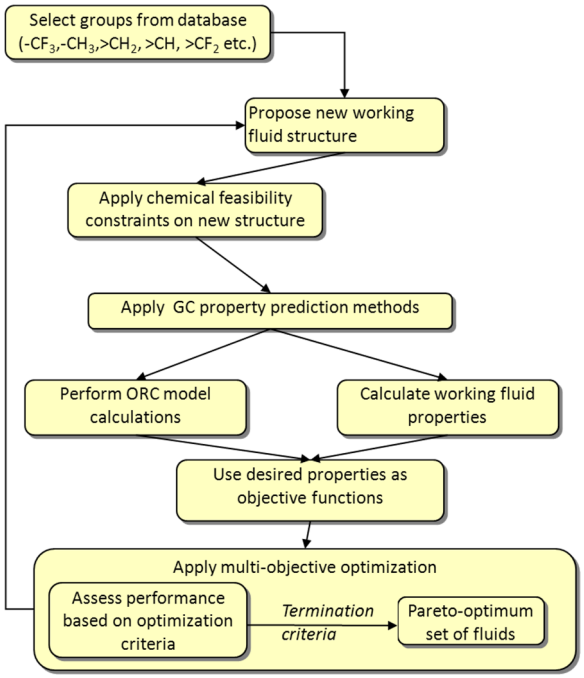

Figure 3. Algorithmic steps involved in the optimization-based CAMD approach used in Papadopoulos *et al.* [4,5].

Papadopoulos *et al.* [4,5,37] consider numerous molecular and ORC process-related properties as performance criteria in an approach which first employs CAMD to design an inclusive set of optimum working fluid candidates and then introduces several of them into ORC process simulations to select few that exhibit favorable process performance. At the CAMD stage properties calculated directly as a result of the working fluid structure involve density, latent heat of vaporization, liquid heat capacity, viscosity, thermal conductivity, melting point temperature, toxicity and flammability. A GC approach has been utilized for their calculation such as the one proposed by Hukkerikar *et al.* [27]. These properties reflect the effects of molecular chemistries on different desired ORC operating and design characteristics. For example, fluids of high density enable equipment of lower volume, fluids of low viscosity enhance the heat transfer hence requiring heat exchangers of lower area, the fluid heat capacity and enthalpy of vaporization have different effects on phase-change and superheating with impacts again on the heat exchanger sizes and cooling loads and so forth. All these properties are considered as objective functions in a multi-objective optimization problem formulation which is solved using Simulated Annealing and results in an inclusive set of Pareto optimum molecules. The development of a Pareto front enables the identification of useful trade-offs among the properties considered as objective functions, while molecules are designed to simultaneously optimize all properties. From a mathematical perspective, in this front no working fluid is of higher performance than the others simultaneously in all properties, but at least one of the properties of a working fluid is better than the same property of another fluid. At the same time, working fluids with worse performance than others in all properties are eliminated and steered clear of the non-dominated set [18,19,38]. The resulting candidate molecules in the Pareto front are then qualitatively evaluated based on their ozone depletion and global warming potentials

considering structural rules from the literature. Selected molecules are introduced into ORC optimization in a basic system configuration. The aim of the optimization of the ORC process is to identify the heat exchange areas required in the vaporizer and the condenser that enable maximum energy recovery with minimum capital cost. The main findings that also illustrate the benefits of the proposed approach are the following:

- Several designed fluids are known chemicals, documented in the online NIST (www.nist.gov) or other databases, indicating the ability of CAMD to identify fluids which are readily available for utilization.
- Despite their public or commercial availability, many of the fluids obtained from CAMD have not been previously considered for ORC applications, indicating the ability of the method to point towards new design directions, overlooked by trial-and-error methods.
- The fluid 3,3,3-trifluoropropene only differs by a single fluorine atom from 2,3,3,3-tetrafluoropropene which has been commercialized in recent years by an international company [39] as an ORC working fluid, highlighting opportunities to quickly investigate other options which are very similar to the proposed designs.
- The fluid hexafluoropropane also obtained from CAMD has been mentioned in patents [40,41] as an ORC mixture component.
- Several unconventional and possibly novel working fluid structures were also identified combining ether and amine functional groups in fluorinated carbon chains. These groups were later shown to result in high ORC thermal efficiency in a study based on molecular thermodynamics [42] which accounted for the results of Papadopoulos *et al.* [4], among other fluids.

An optimization-based CAMD approach was also proposed by Palma-Flores *et al.* [43] which has similarities and differences with the work of Papadopoulos *et al.* [4,5,37] (overview of main points in Table 1). Palma-Flores *et al.* [43] solve an optimization-based CAMD problem which exploits group contribution methods for prediction of properties and also considers the feasibility of the molecular structures through appropriate constraints. Unlike Papadopoulos *et al.* [4,5] who employ Simulated Annealing as the optimization algorithm, Palma-Flores *et al.* [43] employ a Mixed Integer Non Linear Programming (MINLP) model which is solved with a deterministic optimization solver, namely DICOPT. Palma-Flores *et al.* [43] also solve the problem in two stages; first working fluids are designed using CAMD, while the resulting fluids are then compared in terms of ORC performance using three different process configurations. The CAMD stage is implemented 4 times using different objective functions and resulting in 32 working fluids which are further investigated in the second stage. The authors consider a more extensive set of functional groups than Papadopoulos *et al.* [4,5,37] including different aromatic and halogen options. Papadopoulos *et al.* [4,5,37] excluded these options due to issues with toxicity, ozone depletion and global warming. The findings of Palma-Flores *et al.* [43] seem to justify their exclusion. The objective functions include different combinations of working fluid liquid heat capacity, latent heat of vaporization and Gibbs free energy of formation. The first two properties are associated with heating, cooling and phase change operations in the cycle, while the latter is associated with the stability of the designed working fluids. Upper and lower bounds are implemented for the properties used as objective functions, while bounds are imposed on additional properties including critical pressure and temperature, normal boiling point and fusion temperatures. All bounds are obtained

by investigation of the corresponding properties of some very common fluids previously utilized in ORCs. The authors note that some of the designed compounds have been previously considered in research literature but not as ORC working fluids. The authors use their GC models developed from literature sources to predict the working fluid properties hence they select several of them to compare their own predictions with results obtained from the ASPEN software. The observed deviations are mostly less than 5%, although in few occasions larger deviations are also observed. The designed fluids are then introduced in ORC process simulations considering three different process configurations; the basic ORC configuration, an ORC with an internal heat exchanger for heat recovery and an ORC with turbine bleeding and a direct contact heater. The fluids are evaluated considering their thermal efficiency in the different systems.

Lampe *et al.* [44,45] proposed an optimization-based method for the design of optimum ORC working fluids, namely the continuous molecular targeting (CoMT-CAMD) method (Table 1). Working fluids are designed based on a molecular model which allows the use of physical molecular characteristics as continuous decision parameters in the optimization problem. The molecular model takes the form of the perturbed chain statistical associating fluid theory (PC-SAFT) EoS which considers molecules as chains of spherical segments that interact through van der Waals interactions, hydrogen bonds, and polar interactions. The parameters considered in this work are the segment number and diameter as well as the van der Waals attraction between segments. This physical representation of the working fluid is used to calculate the residual Helmholtz energy which allows the calculation of the vapor-liquid equilibria in an ORC model. In this respect, the use of an EoS allows the direct employment of an ORC process model in fluid design and hence the utilization of a process-related objective function (e.g., ORC power output *etc.*). The resulting working fluids are represented by the optimum values of the segment number, diameter and the van der Waals attraction between segments, while Papadopoulos *et al.* [4,5,37] and Palma-Flores *et al.* [43] obtain optimum molecular structures. The resulting working fluid is therefore hypothetical in the sense that it does not necessarily coincide with a real fluid or satisfy chemical constraints (e.g., zero free bonds *etc.*). The authors address this issue by postulating a mapping stage where the parameters of the optimum working fluid are compared with the parameters of real working fluids contained in a database. The proximity of the optimum working fluid with the database fluids is evaluated based on the expected loss in ORC.

It is worth noting here that an approach for working fluid design and selection which shares similar features to Lampe *et al.* [44,45] has been recently proposed by Roskosch and Atakan [46]. The authors perform a reverse engineering design of the working fluid and a heat pump process (which has similarities with ORC) using a cubic EoS. Fluids are represented continuously in the optimization problem through critical temperature and pressure, acentric factor and liquid heat capacity. The problem is solved using non-linear programming (NLP). The resulting optimum solution is then identified based on its proximity to fluids available in a database. Additional criteria such as pressure limits, coefficient of performance and safety are also considered for the selection of the final fluids from the database. CAMD-based approaches addressing the design of refrigerant fluids and/or systems (which also have some similarities with ORC) have also been proposed by Samudra and Sahinidis [47], Sahinidis *et al.* [48], Duvedi and Achenie [49] using deterministic MINLP-based formulations and Marcoulaki and Kokossis [50] using Simulated Annealing.

Table 1. Main points in existing methods for the optimum design of pure ORC working fluids.

Main Points	Papadopoulos *et al.* [4,5,37] [a]	Palma-Flores *et al.* [43] [c]	Lampe *et al.* [44,45] [b]
Implemented stages	*Stage 1*: CAMD optimizing molecular structure. *Stage 2*: Evaluation of optimum molecules in ORC process optimization.	*Stage 1*: CAMD optimizing molecular structure. *Stage 2*: Evaluation of optimum molecules in ORC process simulation.	*Stage 1*: CoMT-CAMD optimizing molecular parameters and ORC process. *Stage 2*: Mapping of optimum molecular parameter values in molecular structures of existing molecules.
Property prediction method	GC + EoS; (e.g., standard cubic)	GC + EoS; (e.g., standard cubic)	PC-SAFT + QSPR (for ideal heat capacity)
Working fluid optimization parameters (*Stage 1*)	Functional groups (discrete, result in optimum structure)	Functional groups (discrete, result in optimum structure)	Segment number, diameter and van der Waals interactions (continuous, result in optimum values)
Optimization approach (*Stage 1*)	Multi-objective optimization, Simulated Annealing	Single objective optimization, MINLP solver	Single objective optimization, NLP solver
Working fluid optimization criteria (*Stage 1*)	Density, Enthalpy of vaporization, Liquid heat capacity, Viscosity, Thermal conductivity, Toxicity, Flammability, Melting point temperature, Critical temperature, Ozone depletion potential (qualitative), Global warming potential (qualitative).	Enthalpy of vaporization, Liquid heat capacity, ratio of the two, weighted sum of the two and the standard Gibbs energy of formation of an ideal gas.	ORC net power output.
Optimization criteria (*Stage 2*)	Unified index considering maximization of power output revenues and minimization of capital costs (vaporizer and condenser areas).	ORC thermal efficiency.	Expected loss in process performance of optimum (theoretical fluid) compared to real fluids in a database.
Identified fluids [a]	• CF_3-CH_2-CF_3 (Hexafluoropropane-R236fa) • CF_3-CH=CH_2 (Trifluoropropene-R1243) • CH_3-CH_2-CH_3 (Propane) • CH_3-O-NH-CH_3 • NH_2-CH_2-O-CH_3 • $HCOOCH_3$ • FCH_2-O-O-CH_2F • CH_3-O-O-CH_3	• CH_3-O-N(OH)-CH_3 • NH_2-O-CH_2-F • CH_3-CH_2-COO-CH_2-F • Cl-COO-CH_2-CH_3 • CH_3-O-O-N(F)-OH	• CF_3-CHF-CF_3 (Heptafluoropropane-R227ea) • CF_3-CH=CH_2 (Trifluoropropene-R1243) • CH_3-CH_2-CH_3 (Propane)

Heat source temperatures: [a] 90 °C, [b] 120 °C, Evaporator working fluid outlet temperature: [c] 190 °C.

3.4. Optimization-based CAMD of Mixtures

The design of mixtures is a considerably more challenging problem than the design of pure fluids; it requires the determination of (a) the optimum number of working fluids in the mixture, (b) the optimum

mixture composition (*i.e.*, the structure of each mixture component) and (c) the optimum mixture concentration (*i.e.*, the amount of each component in the mixture). Papadopoulos *et al.* [18,19] proposed for the first time the design of binary ORC working fluid mixtures through a novel, optimization-based CAMD approach which may also be used for the design of mixtures in other applications. The proposed approach involves two main stages which are illustrated in Figure 4. The first stage aims to explore and identify the highest possible economic, operating, environmental and safety performance limits of a wide set of mixtures in an ORC system. This is approached in Stage 1 by searching for chemically feasible fluid structures only for one of the two components (*i.e.*, the 1st) of a binary mixture, while emulating the mixture behavior of the 2nd component within a much wider structural design space by lifting the chemical feasibility constraints. Note that in each stage the proposed approach enables the simultaneous mixture and ORC design. The two stages interact to help improve the performance of the obtained solutions. The proposed approach builds on the previous work of Papadopoulos *et al.* [4,5,37] for CAMD-based design of pure fluids hence the identification of multiple optimum mixture candidates is again accomplished through a multi-objective formulation of the CAMD-optimization problem, treating multiple ORC performance measures simultaneously and resulting in a comprehensive Pareto front revealing useful structural and property trade-offs among mixture components. Stage 2 serves to determine the optimum and chemically feasible structure of the 2nd component for each one of the feasible fluids (1st components) already obtained in Stage 1, together with the optimum mixture concentration. In Stage 2, the mixture performance limits identified in the previous stage are used as a reference point to efficiently avoid sub-optimal choices. The design of binary mixtures could in principle be approached directly in Stage 1 (*i.e.*, without the need for a second stage) by implementing chemical feasibility constraints on both new fluid structures. However, this may require increased computational effort, especially if such an approach is extended to mixtures of more than two components. Instead, the effort is reduced in the proposed approach as the user is allowed to review, interpret and analyze the rich intermediate insights generated by the multi-objective optimization approach prior to exploiting meaningful conclusions between design stages. Optimum solutions are identified in a Pareto sense, enabling the exploitation of the often conflicting design objectives. Some of the resulting mixtures are shown in Table 2, containing fluids that also favor the ORC performance even when they are used as pure fluids.

An approach addressing the optimization of working fluid mixtures for ORC is presented in Molina-Thierry and Flores-Tlacuahuac [51]. The number of working fluids participating in the mixture, the type of working fluids that form the mixture and the mixture concentration are optimized together with the ORC operating conditions. The working fluids that are used to perform mixture combinations are selected from a pre-specified set of three, eleven or six pure fluids in the performed case studies. This is different to Papadopoulos *et al.* [18,19] who identify the optimum structure of both working fluids participating in binary mixtures, simultaneously with the ORC operating conditions and without having a set of pre-specified options.

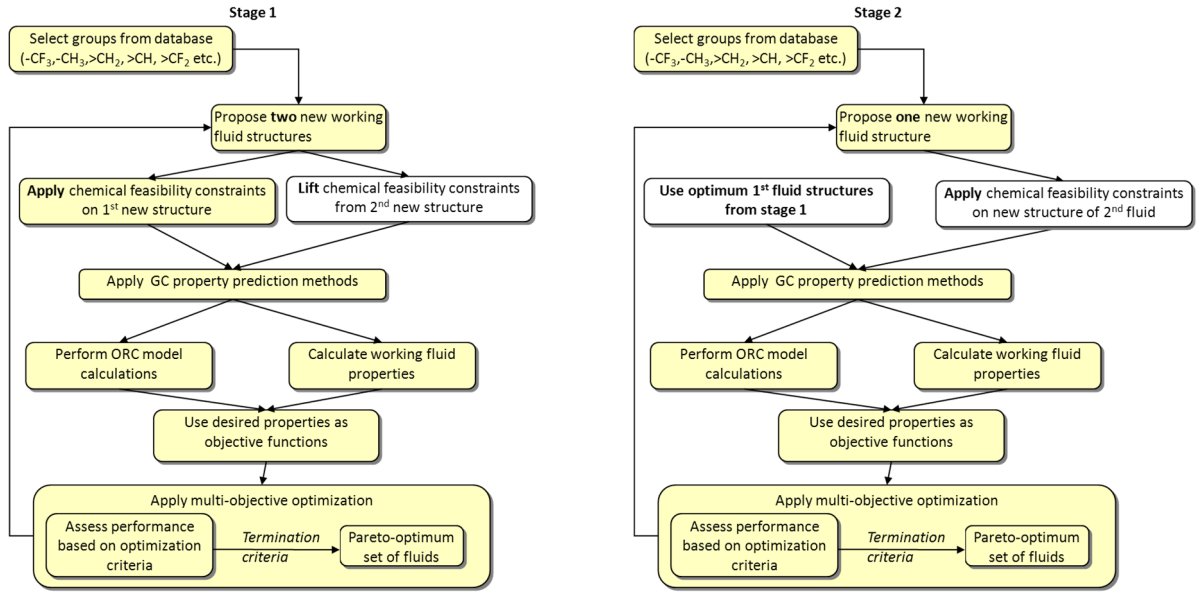

Figure 4. Algorithmic steps involved in the optimization-based CAMD approach for simultaneous mixture and ORC design used in Papadopoulos *et al.* [18,19].

Table 2. Main points in methods for optimum design and selection of ORC working fluid mixtures.

Main Points	Papadopoulos *et al.* [18,19] [d]	Molina-Thierry and Flores-Tlacuahuac, [51] [e]
Implemented stages	*Stage 1*: CAMD optimizing 1st and theoretical 2nd structure, concentration and ORC process. *Stage 2*: CAMD optimizing 1st and 2nd structure, concentration and ORC process.	Optimizing number and type of working fluids in mixture (generated from a pre-specified set of pure fluids), mixture concentration and ORC process.
Property prediction method	GC + EoS (e.g., standard cubic)	GC + EoS (e.g., standard cubic)
Working fluid optimization parameters (*Stage 1*)	Functional groups (discrete, result in optimum structure), concentration (continuous)	Preselected set of pure fluids used to form mixture combinations (discrete), concentration (continuous)
Optimization approach (*Stage 1*)	Multi-objective optimization, Simulated Annealing	Single objective optimization, testing of several objectives, MINLP solver
Working fluid and process optimization criteria (*Stage 1*)	Exergetic efficiency, thermal efficiency, flammability of each fluid, mixture maximum and minimum flash points (constraint), mixture azetropic concentration (constraint).	Change of the enthalpy of vaporization at the cycle high pressure level, specific net work output, first and second law efficiency, area in between profiles (temperature-enthalpy) of the working fluid and heat source or sink on the heat exchanger
Optimization criteria (*Stage 2*)	Same as *Stage 1*	Not applicable
Uncertainty in mixture selection	Considered through a systematic non-linear sensitivity analysis approach	-
Identified fluids	• CF_3-CH_2-CH_3/FCH_2-O-$(CH_2)_2$-CH_3 • CF_3-CH_2-CF_3/FCH_2-O-CH_2-CF_3 • (CH_3)-C/FCH_2-O-C-$(CH_3)_3$	• RC318 (refrigerant)-*n*-Pentane (case B) • R245ca- *n*-Pentane (case B) • FC4-1-12-*n*-Butane (case C)

Heat source temperatures: [d] 90 °C, [e] 90–150 °C.

The authors present details on the employed ORC model which involves vapor-liquid equilibrium and other calculations using models similar to Papadopoulos *et al.* [18,19]. They employ a single objective formulation, trying five different simple or complex objective functions during optimization and considering three different case studies. The optimization results in the same binary mixture components in the first case study, with changes observed only in the mixture concentration depending on the employed objective function. In the second case study the authors use the first law efficiency as an objective function and solve the optimization problem for several different heat source temperatures. The mixture compositions and concentrations change significantly. Although in some cases the results indicate mixtures consisting of four components, only two of them are in significantly high concentration, the remaining two are traces. The third case study addresses the optimization problem independently for two objective functions indicating that the choice of the objective function affects both the optimum mixture characteristics (composition, concentration) and performance. One case finds a binary mixture as the optimum solution, while the other finds a mixture consisting of five working fluids in significant concentrations. The obtained mixtures are not comparable with Papadopoulos *et al.* [18,19] because the latter used different functional groups. The authors note that in the future they will also consider uncertainty as well as process control (discussed in the subsequent sections).

3.5. Uncertainty in Predictions

The use of predictive models for the calculation of working fluid or ORC process properties involves uncertainty regarding the accuracy of the obtained predictions. Uncertainty is mainly observed in the employed GC, thermodynamic or process models and results in over- or under- estimation of the predicted thermodynamic or process behavior of the investigated or designed fluids. The use of different prediction models or input parameters for the calculation of the same property may result in values that deviate. While deviations may be significant for particular fluids, others may exhibit similar property values regardless of the employed property prediction model. Lampe *et al.* [45] illustrate the impact of the working fluid structure on the ORC net power output through their continuous molecular representation using the geometric and interaction parameters. The reported three-dimensional diagram indicates areas with very steep non-linear changes as well as areas with smoother changes. In other words, the sensitivity of the employed model under the influence of different fluids may vary significantly. In the case that experimental measurements are available it is possible to determine the accuracy of the predictive models and hence ensure that by accounting for predictive inaccuracies the designed or selected fluids represent realistic ORC performance options. However, experimental measurements exist for very few working fluids under very specific conditions. It is therefore necessary to utilize a systematic method which enables the validation of the obtained predictions with respect to their expected accuracy, regardless of the availability of experimental measurements or the predictive capability of the available models.

Papadopoulos *et al.* [18,19] proposed a sensitivity analysis approach which facilitates the identification of parameters with high influence in the overall working fluid-ORC system performance, the quantification of the overall system sensitivity with respect to these parameters and the incorporation of sensitivity metrics during the decision-making involved in the optimum working fluid selection. The proposed method identifies ORC process performance areas that present steeper or smoother changes for different fluids under the simultaneous influence of multiple different parameters for each fluid and

determines the parameters with the highest influence in the changes. The method was implemented in the selection of optimum ORC working fluid mixtures and may be also be used for the selection of pure working fluids. It is based on the development of a sensitivity matrix which incorporates the derivatives of the ORC performance measures (e.g., thermal or exergetic efficiency *etc.*) with respect to model parameters and constitutes a measure of the variation of the employed model under the influence of infinitesimal changes imposed on model parameters. The sensitivity matrix is decomposed into major directions of variability to identify the largest in magnitude eigenvector. This represents the dominant direction of variability for the system, causing the largest change in the performance measures. The entries in the dominant eigenvector determine the major direction of variability in the multiparametric space and indicate the impact of each parameter in this direction. Having identified this direction it is not necessary to explore all directions of variability (*i.e.*, combinations of parameters) arbitrarily hence reducing the dimensionality of the sensitivity analysis problem. The dominant eigenvector is then exploited in a sensitivity index which accounts for all performance indices simultaneously within a wide variation range explored also through an appropriate parameter. In this respect, the optimum working fluid mixtures which resulted from CAMD were also evaluated in terms of the accuracy in the performance predictions. Some mixtures that exhibited high ORC performance seemed to be very sensitive in changes in certain model input parameters; in case that these parameter values are not sufficiently accurate the predicted performance will drop significantly. The predicted performance of several other mixtures that exhibited low sensitivity would not be affected even if the model input parameter values were less accurate.

3.6. Simultaneous vs. Integrated Design Approaches

The reviewed cases reveal that the design and/or selection of working fluids follows two major approaches:

- An approach that supports the *simultaneous* working fluid and ORC design and/or selection (Palma-Flores *et al.* [43]; Lampe *et al.* [44,45]; Papadopoulos *et al.* [18,19]; Molina-Thierry and Flores-Tlacuahuac [51]).
- An approach that supports the *integrated* working fluid and ORC design and/or selection (Papadopoulos *et al.* [4,5,37]).

In most of the above cases the pure or mixed working fluid structure(s) are designed using a CAMD approach. There is also an option of determining an optimum pure working fluid or the mixture composition and concentration from a pre-specified list of working fluids (of known structures) or their combinations. This may be done either through a *simultaneous* or an *integrated* approach.

- The meaning of *simultaneous* is that decisions regarding the working fluid structure, composition or concentration (in case of mixtures) are taken within the same optimization algorithm that identifies the optimum ORC operating and/or sizing characteristics. The advantage of a *simultaneous* approach is that the working fluid and ORC interactions are accounted for together and drive the optimization search to identify an optimum solution. This is reasonable because a working fluid is an inherent component of the ORC system in which it is utilized. However, simultaneous approaches may suffer from combinatorial complexity if the design options in both

the working fluid and ORC sides are extensive. The relevant reviewed works incorporate a basic ORC structure into working fluid design in order to identify fluids directly based on their impact in the ORC process. It would be ideal to also consider the structural characteristics of the ORC (e.g., recuperation, pressure levels *etc.*) simultaneously with working fluid design but this would lead to an intractable optimization problem due to the vast number of potential options and the non-linearities of the employed models. For example, Palma-Flores *et al.* [43] consider more complex ORC structures in simulations performed after the optimum working fluids were identified.

- The meaning of an *integrated* design approach is that working fluids are first designed using fluid properties as objective functions and the obtained fluid(s) are then introduced in a full ORC model simulation or optimization, as in the case of pure fluid design presented in Papadopoulos *et al.* [4,5]. *Integrated* design approaches evolved from the need to decompose the CAMD and process design problems so that an extensive search space (e.g., working fluid and process structures, operating parameters *etc.*) may be considered within reasonable computational efficiency. The key to the efficient integration of a CAMD and a process design stage is to identify the working fluid(s) that will subsequently facilitate high performance in ORC optimization, while avoiding the premature exclusion of useful fluid options. In a broader sense *simultaneous* approaches could become part of the problem decomposition rationale employed in *integrated* approaches. This is because at some point optimum working fluids and process characteristics obtained from the *simultaneous* design stage will have to be transferred to a subsequent, independent design stage to perform optimizations either using more detailed and realistic models or exploring a much wider design space. *Integrated* approaches address the problem of obtaining and transferring useful and inclusive design information in the subsequent stage.

Table 3. Merits and shortcomings of considered methods and objective functions in fluids design.

	Merits	**Shortcomings**
Fluid selection from a pre-specified list	Few options to investigate in an optimum selection problem of reduced size, ORC model may be used, selection may also be based only on molecular properties, commercially available fluids may be used directly	The consideration of few options limits the search, arbitrarily excluded working fluids may be the ones that maximize ORC performance, novel working fluids may not be identified
Simultaneous design methods	Directly link molecular characteristics with ORC process performance, novel working fluids may be identified	Require an ORC model, which may however reduce computational efficiency if modeling rigor is increased
Integrated design methods	Enable the consideration of a more extensive design space and/or more detailed models in each design stage, maintain manageable computational effort, novel working fluids may be identified	Require efficient integration between stages to avoid excluding important designs early on in the search
Molecular properties as objectives	Easy to calculate and implement through GC methods, no need for an ORC model, appropriate for CAMD and multi-objective formulations	Indirectly reflect on ORC process performance characteristics, not appropriate for use in single-objective formulations

Table 3. *Cont.*

	Merits	Shortcomings
ORC process performance indices as objectives	Directly link CAMD with ORC performance, provide associations with cost/profit characteristics (e.g., net generated work) or direct use of them, support more realistic solutions when more detailed models are used	Detailed ORC models may impact on computational efficiency, associations to cost/profit through less detailed models may be limited to specific ORC characteristics, overlooking other important costs, depending on the model detail
Single-objective formulations	Easy to implement, result in a single optimum solution	The use of different properties as the objective function is likely to result in different optimum working fluids
Multi-objective formulations	Handle multiple and often conflicting objectives simultaneously, result in a rich set of working fluids, appropriate for molecular properties	More difficult to implement than single-objective formulation

Table 3 provides an overview of merits and shortcomings. Note that *simultaneous* and *integrated* approaches are not related to the type of the employed optimization algorithm which may either be stochastic such as Simulated Annealing *etc.* (Papadopoulos and Linke [52]) or deterministic such as NLP- or MINLP-based algorithms *etc.* (Cavazzuti [53]) in both cases. Optimization algorithms are discussed in the next section.

3.7. Single- vs. Multi-objective Optimization and Types of Objective Functions

Regardless of the employed approach, molecular properties are often used as working fluid screening or design criteria because they indirectly reflect on ORC process performance. For example, high working fluid density may enable a reduction in the required fluid amount hence equipment of lower size may be used. High thermal conductivity enables heat exchangers of lower areas and so forth. In *single-objective* optimization formulations the use of a molecular property as objective function may lead to optimum working fluids which are different depending on the selected property. They may also be different to the results obtained from a simultaneous approach. These challenges are best addressed by the use of a *multi-objective* optimization formulation in the working fluid design stage (Table 3). In such a case:

- There is no need to select one of the properties as an objective function in order to guide CAMD into the identification of a single optimum molecule, while there is no need to set upper and lower bounds (which are often not known a priori) in the remaining properties which are used as constraints. This is very important because there are many working fluid properties that may be considered as objective functions and a *multi-objective* formulation does not have limitations on how many may be included.
- Such an approach results in a Pareto front which consists of many working fluids, instead of one obtained in a *single-objective* case. The Pareto fluids represent multi-fold and rich trade-offs in the entire ORC performance spectrum. They can be incorporated as discrete options in a subsequent comprehensive ORC design stage (see next section) where the optimization and computational efficiency remain manageable (Papadopoulos and Linke [16]).

As shown in Table 1 the optimum working fluids obtained from the integrated design approach of Papadopoulos *et al.* [4,5] are very similar to those obtained by the simultaneous approach of Lampe *et al.* [44,45]. Papadopoulos *et al.* [4,5] were able to capture such working fluids without the use of an ORC model in the course of working fluid CAMD (hence the computations were fast) due to the use of multiple property objective functions. Note that the results are comparable because the heat source temperatures are quite close and the fluids are pure. Papadopoulos *et al.* [37] reported that for heat source temperatures between 70–90 °C the rank ordering of working fluids in terms of ORC performance remained the same. Similar findings with respect to the selected fluids have been previously reported by Papadopoulos and Linke [38] who compared a simultaneous and an integrated *multi-objective* CAMD approach in a different application (*i.e.*, solvents for industrial separations).

The type of properties that could be used as objective functions in a single- or multi-objective CAMD working fluid formulation have been thoroughly discussed in Stijepovic *et al*. [17], while insights have also been discussed in Papadopoulos *et al*. [4] and Palma-Flores *et al*. [43].

In the case of pure fluids:

- Stijepovic *et al.* [17] investigated the impact of different working fluid properties in the cycle thermal, exergetic efficiency and economics as a function of heat transfer areas and net generated work. It was found that high values of fluid compressibility factor and low values of saturated liquid molar volumes favor all three criteria. Fluids of high molecular weights favor thermal efficiency and of high isobaric heat capacities favor exergetic efficiency and economic performance, whereas low enthalpy of vaporization also favors the same criteria. Low critical pressure, high saturated liquid thermal conductivity and saturated gas volume favor economic performance.
- Palma-Flores *et al.* [43] report that the molecules resulting from minimization of liquid heat capacity and of a complex objective that combines a weighted sum of enthalpy of vaporization, liquid heat capacity and standard Gibbs energy of formation of an ideal gas result in higher thermal efficiency and work output.

In the case of mixtures:

- Papadopoulos *et al.* [18] finds that exergetic efficiency increases at a higher rate than thermal efficiency decreases, as the concentration moves from pure component to approximately equal amounts of components in the mixture. The use of a multi-objective approach appears helpful.
- Molina-Thierry and Flores-Tlacuahuac [51] find that the first law efficiency is the most appropriate objective to use in a single objective formulation.

Note that objective functions associated with costs are clearly useful but difficult to use when the goal is to design or screen for efficient working fluids. Even when an ORC model is used as part of working fluid design it is mainly based on a thermodynamic representation which indirectly associates cost with indices like net generated power. Papadopoulos *et al.* [4] note that about 90% of process costs are associated with heat exchangers. Although it would be desirable to calculate heat exchanger areas in the course of working fluid design, it is not practical mainly due to data limitations (e.g., heat transfer coefficients *etc.*). Furthermore, there are also numerous and complex economic performance indices which influence the optimum solution but are impractical to use in working fluid design due to limitations in the rigor of the employed model. Kasaš *et al.* [54] note that only those process models with

sufficient levels of accuracy are suitable for generating proper optimal designs using the correct economic criterion. Such issues are discussed in the next section.

4. Optimization Approaches for Organic Rankine Cycles

4.1. Main Concepts and Computational Challenges

The careful selection of the working fluid is instrumental to the performance of the ORC as discussed above. Equally importantly, an ORC process configuration needs to be determined to enable efficient power generation for the given heat source(s). In addition, the cycle operating conditions need to be set such that the chosen performance criterion is maximized. The overall design problem requires discrete decisions on the selection of structural design alternatives such as alternative heat exchanger options or selection of the number of cycles to integrate as well as optimization of the continuous variables associated with operating conditions and equipment sizes. Systematic approaches can aid the exploration of the design options to guide the identification and selection of efficient overall designs. The computational challenges are similar to those observed in working fluid design. A very large number of structural and operating options need to be considered as part of the ORC flowsheet in order to identify an optimum system of high efficiency, whereas sufficiently accurate process models are also required so that the obtained designs are realistic. The three general model types that may be considered for the design of ORCs involve (Figure 5):

(a) Computational fluid dynamic (CFD) models for detailed equipment design [55].
(b) Process level models that incorporate thermodynamic calculations with equipment details for equipment sizing within the flowsheet.
(c) Thermodynamic cycle models which account for energy balances and phase change operations.

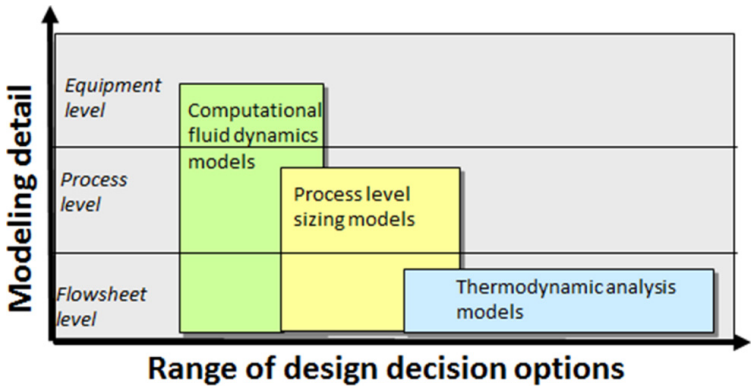

Figure 5. Equipment, process and flowsheet models with respect to modeling detail and range of design decision options which may be simulated at a reasonable computational effort.

The simultaneous utilization of representatives from all model types would be ideal but computationally impractical. Each model type may be used independently but not all types are suitable for the optimum design of ORC flowsheets. CFD models capture local heat and/or mass transfer phenomena within the equipment with great detail, but the computations are time consuming. Process level sizing models enable the consideration of economic performance measures to evaluate different flowsheet alternatives and allow the consideration of an increased range of decision options within

reasonable computational efficiency. However, the use of such models in the course of working fluid design or selection (*i.e.*, with the molecular structure as an additional design parameter) may be limited by the lack of data (e.g., prediction models of heat transfer coefficients for different working fluids are quite complex [56]) and by the high combinatorial complexity of the design problem. Finally, thermodynamic analysis models enable the consideration of a much wider range of process and flowsheet design decision options, they have been used in the course of working fluid design as shown in the previous section and provide useful insights about different ORC flowsheet configurations prior to proceeding into a more rigorous evaluation.

The literature is abound with works that explore cycle operating conditions and structures largely through sensitivity analyses via repeat simulation studies to identify efficient settings for selected designs and given heat sources and sinks. The limitation of such contributions lies in the need for prior knowledge of an ORC configuration which may lead to good performance. Although empirical knowledge is very useful, the trial-and-error testing of different ORC configurations is likely to enable incremental performance improvement. Such contributions will not be reviewed here; instead, we will limit our focus to emerging systematic approaches to design efficient ORC systems. A number of such optimization-based approaches have been proposed in the last few years. The general ORC design optimization problem for such approaches can be stated as: *Given a heat source stream and ambient conditions, determine the optimal cycle configuration and design parameters that maximize ORC performance with respect to chosen performance criteria*. Notice that in this formulation it is not necessary to pre-specify an ORC structural or operating profile that will be optimized. Structural and operating ORC parameters may become decision variables in an optimization search which is guided toward the optimum solution by the chosen performance criteria through an algorithmic sequence. This does not eliminate the need for empirical knowledge which may be used to focus the design space into significant decision options or to interpret the design results in terms of their practical applicability. Earlier works focus at optimizing the design and/or operating parameters of ORC systems, whilst the most recent contributions attempt to consider alternative configurations in optimization approaches.

4.2. Reviewed Approaches

The reviewed works are organized into three categories based on the way that the cycle and working fluids are selected (Tables 4–6). Franco and Villani [57] were amongst the first to present an optimization scheme to help the identification of efficient design parameters for an ORC in a binary geothermal power plant. They propose to decompose the ORC optimization problem into three subsystems, the heat recovery cycle, the heat recovery exchanger and the cooling section. The three subsystems are evaluated in an overall iterative scheme where operating characteristics of the cycle are determined based on the optimization of the heat recovery and cooling system sizes. The performance measures are the first and second law efficiencies as well as the brine consumption from implementation of the system for a geothermal heat source. Six pre-selected working fluids are considered together with three ORC structures (supercritical, dual pressure level, ORC with superheater) which are all evaluated. Details on the implementation of the optimal search and convergence properties have not been provided.

With a different application focus, Salcedo *et al.* [58] propose a multi-objective optimization formulation for an integrated system of a solar ORC and a reverse osmosis desalination plant. The

approach allows to explore the equipment sizes and operational conditions of a predefined system configuration and considers two objectives: Cost of water produced and the life cycle global warming potential. The resulting MINLP problem is solved by exhaustive enumeration using a deterministic nonlinear optimization algorithm. With respect to a standard ORC configuration, Wang *et al.* [59] propose an optimization approach to determine optimal design parameters using global search schemes in the form of meta-heuristics. The approach allows one to determine the optimal turbine inlet pressure and temperature as well as temperatures against heat sources and sinks. The ratio of net work to heat transfer as an indicator of cost is maximized as the design objective. A Genetic Algorithm is implemented to solve the nonlinear continuous optimization problem.

Table 4. Cycle operating/sizing parameters are optimized for different, pre-determined cycle structure and working fluid combinations.

Authors	Optimization Approach	Decision Parameters	Objective Functions
Franco and Villani [57]	Iterative hierarchical identification of optimum ORC size and operating parameters for each combination	Six pure working fluids, sizes of cooling systems and recovery heat exchanger, three cycle structures (supercritical, dual pressure level, ORC with superheater)	First, second law efficiency, brine consumption
Salcedo *et al.* [58]	MINLP problem, deterministic nonlinear algorithm	Equipment sizes, operating conditions, one cycle structure	Cost of water produced in desalination plant, global warming potential
Wang *et al.* [59–61]	Genetic algorithm [59,62], multi-objective genetic algorithm [60,61]	Turbine inlet pressure and temperature, temperatures against heat sources and sinks [59,60], geometry of ORC heat exchanger [61], one cycle structure	Net power output to total heat transfer area [59], exergetic efficiency and capital cost [60], pressure drop, heat transfer area [61]
Xi *et al.* [62]	Genetic Algorithm	Three regenerative cycle structures, six pure working fluids, operating parameters	Exergetic efficiency
Walraven *et al.* [63,64]	Deterministic NLP	Eight pure working fluids, tube diameters, baffle spacing in heat exchangers, two different cycle structures	Levelized cost of electricity [63], net present value [64]
Victor *et al.* [30]	Simulated Annealing	Composition of working fluid mixture, ORC, Kalina cycle	Thermal efficiency

Wang *et al.* [60] later proposed the solution of a problem considering two objectives simultaneously, the exergetic efficiency and the capital cost. The Pareto frontier is determined using a multi-objective Genetic Algorithm. Xi *et al.* [62] propose a Genetic Algorithm based approach for parameter optimization of regenerative ORC configurations to achieve maximum exergetic efficiency.

The application of the approach is illustrated with a study of three different cycle configurations and six different working fluids in an exhaustive search. At the level of equipment design, Wang *et al.* [61] optimize the geometry of ORC plate heat exchanger condensers using a multi-objective Genetic Algorithm to explore the nondominated solutions with respect to pressure drop and heat transfer area.

Walraven *et al.* [63] present a parameter optimization scheme for single and multi-pressure ORCs that takes into account the geometry of shell-and-tube heat exchangers for the heat recovery section as well as models for dry cooling. Multi-pressure ORCs are represented by flowsheets where the working fluid is compressed in two or more loops at different temperature levels. Dry cooling refers to air cooled condensers. In contrast to the more prominent global search algorithms based on meta-heuristics, the optimization problem is solved using a local deterministic NLP solver to determine the optimized ORC design parameters such as tube diameters and baffle spacing that yield the maximum Net Present Value of the system. Structural variants are again explored through repeat solutions of pre-selected configurations. Earlier, Walraven *et al.* [64] presented a similar optimization scheme that uses the Levelized Cost of Electricity as the objective function taking into consideration wet and air cooling. Wet cooling refers to a water-cooled tower.

Moving beyond pure component working fluids, Victor *et al.* [30] consider ORCs and Kalina cycles with working fluid mixtures and propose an optimization approach to determine the optimum working fluid composition that maximizes the thermal efficiency of the cycle. The optimization problem is implemented using the Simulated Annealing meta-heuristic to perform a global search of the solution space.

Gerber and Marechal [65] proposed a multi-period, multi-objective optimization approach to determine optimal configurations for geothermal systems while accounting for seasonality. Multi-period optimization is used to enable the incorporation of parameter variation in the design procedure. The optimization is based on the expected value of the objective function for a given parameter variability. Usually, parameter variation is imposed through the consideration of multiple parameter realizations taken from the selected parameter space as discrete instances of the plant (periods) [66]. The overall approach employs an evolutionary algorithm across the multiple periods considered and draws on process integration approaches and the solution of single period mixed-integer linear programming (MILP) problems to determine the optimal configurations with respect to objective functions including the investment and operating cost and the exergetic and energetic efficiency. The problem involves the selection or combination of different energy technologies for the exploitation of geothermal fields at different depths. Among other technologies, two ORCs are considered, one single-loop and one with intermediate draw-off. The decision parameters for the ORCs involve the evaporation and saturation temperature in both cases as well as draw-off split fraction and condensation temperature in the second case.

Taking into account structural ORC design decisions, Pierobon *et al.* [67] propose an optimization approach to simultaneously explore design parameters and structural alternatives for ORC configurations and single working fluid options from a predefined set of candidates. The approach implements a Genetic Algorithm to simultaneously explore the design space for three objective functions: The Net present Value, the total system volume and thermal efficiency. The approach simultaneously determines the best working fluid from a predefined set, sizes the heat exchangers, and determines the temperature and pressure settings of the cycle. Larsen *et al.* [68] present a variation of the work to simultaneously explore alternatives for ORC configurations in terms of internal heat recovery and superheating options. A data set of 109 working fluids is screened before the optimization based on thermodynamic and hazard criteria. Few working fluids are optimized simultaneously with the ORC structural and operating options. Both works study waste heat recovery on an offshore platform to illustrate the approach.

Most recently, Clarke and McLeskey [69] have proposed a multi-objective optimization approach for ORC system design. Their approach allows to simultaneously consider two objective functions, the specific work output of the ORC and the specific heat exchanger area, and six decision variables: The choice of alternative working fluids out of a predefined set of 17 candidates, the evaporation temperature, the minimum approach temperature, the effectiveness of the superheater, the effectiveness of the recuperator and the temperature difference in the condenser. The Pareto front is developed using a Particle Swarm optimization algorithm which has been implemented for geothermal power generation. The benefit from the optimization tool in exploring the design options is highlighted.

Table 5. Optimum cycle structure, operating/sizing parameters and working fluids are selected simultaneously from a pre-determined set of options.

Authors	Optimization Approach	Decision Parameters	Objective Functions
Gerber and Marechal [65]	Multi-period, multi-objective, evolutionary algorithm across multiple periods, MILP in single periods (cycle structure and operation)	Two cycle structures (single-loop, intermediate draw-off), evaporation and saturation temperature (both structures), draw-off split fraction and condensation temperature (2nd structure)	Investment and operating cost, exergetic and energetic efficiency
Pierobon *et al.* [67]	Genetic algorithm (cycle operation and working fluid)	Five pure working fluids, size of heat exchangers, turbine inlet pressure and temperature, the condensing temperature, pinch points, superheating temperature difference, target velocities in heat exchangers	Thermal efficiency, total system volume, net present value
Larsen *et al.* [68]	Genetic algorithm (cycle structure, operation and working fluid)	Set of working fluids, structures with recuperation and/or superheating	Thermal efficiency
Clarke and McLeskey [69]	Multi-objective particle swarm (cycle operation and working fluid)	Seventeen working fluids, evaporation temperature, minimum approach temperature, effectiveness of superheater and recuperator, temperature difference in condenser	Specific work output, specific heat exchanger area

The methods presented thus far aim at the optimization of fixed ORC configurations with a pure working fluid. In a recent attempt to broaden the search towards including a broader set of structural design candidates, Stijepovic *et al.* [70] propose a method for the optimal design of multi-pressure ORCs to generate power form a single heat source stream. The approach draws on the Exergy Composite Approach by Linnhoff and Dhole [71] to formulate an optimization problem that is repeatedly solved to determine the ORC configuration and its optimal operating conditions with minimum exergy loss and maximum work output. The work considers both induction and expansion turbines. The presented results highlight significant performance improvements of the developed multi-pressure ORC configurations over the standard single-pressure ORC configuration. Toffolo [72] proposes an optimization approach to determine optimal configurations and design parameters for ORCs that absorb and release heat at different temperatures. The approach combines a Genetic Algorithm (GA) to screen configurations with a sequential quadratic programming (SQP) approach to determine design parameters. It is based on a generic flowsheet representation which may be used to determine different topologies including different numbers of pressure and expansion levels as well as heat exchange operations.

Table 6. Optimum cycle structure and operating/sizing parameters evolve during the optimization search; the optimum cycle structure is not pre-determined but results from optimization.

Authors	Optimization Approach	Decision Parameters	Objective Functions
Stijepovic *et al.* [70]	Iterative addition of pressure loops to optimize an evolving structure, deterministic NLP inside each loop to optimize the operating parameters	Number of pressure loops, working fluid flowrates, saturation temperatures, evaporator outlet temperatures per loop, two expandable multi-pressure ORC configurations, type of turbine (induction, expansion)	Exergy loss, work output
Toffolo [72]	Genetic algorithm to synthesize structure, sequential quadratic programming to optimize objective function	Number and configuration of pressure loops, expansion and heat exchange stages	Net generated electrical power

4.3. ORC Process Structure Classes and Types

In summary, the past five years have seen the emergence of optimal design approaches for ORCs. Based on the performed review these approaches may be broken down into three general classes:

- *Fixed flowsheet approaches*: Those that focus on parameter optimization as well as on addressing equipment design decisions for a pre-specified ORC flowsheet.
- *Flowsheet selection approaches*: Those that consider cycle operating and equipment design for different pre-specified flowsheets. In such cases the pre-specified flowsheet structures may be decision parameters in the optimization or each structure may be optimized separately, one-by-one in terms of operating and equipment characteristics.
- *Flowsheet design approaches*: Those that have broadened the scope towards the inclusion of structural design decisions within the cycle. In such cases the flowsheet structure is not entirely pre-specified but a flexible structure gradually evolves into different configurations and the optimum flowsheet results from the optimization, together with operating and equipment characteristics.

This trend is expected to continue to yield systematic design approaches that can simultaneously consider the design parameters together with structural design alternatives associated with multiple working fluids, multiple integrated cycles and multiple pressure levels. The availability of such methods will be instrumental to the quick determination of optimal ORC-based power generation schemes for any given heat source and sink. A recent review by Lecompte *et al.* [73] provides an elaboration of several ORC structures studied in literature, based on the goals that they intend to address:

- Structures that intend to decrease irreversibility and match the temperature profiles between heat source and the working fluid involve transcritical cycles, trilateral cycles, cycles with zeotropic mixtures as working fluids, cycles with multiple evaporation pressures, organic flash cycles and cascade cycles.
- Structures that intend to increase thermal efficiency by maximizing the mean temperature difference between heat addition and heat rejection involve cycles with the addition of a recuperator, Regenerative cycles with turbine bleeding, cycles with reheaters and cycles with vapor injector.

4.4. Stochastic vs. Deterministic Optimization Methods

The key practical issues to be considered in the selection of an appropriate optimization method are the existence of integer and/or continuous design variables, of non-linearities (e.g., convexities or non-convexities) in the employed working fluid or ORC models and the quality of the obtained solutions (globally *vs.* locally optimum solutions). The two main existing categories are *deterministic* and *stochastic* optimization methods [53] (Table 7).

- *Deterministic* optimization methods exploit analytical properties (e.g., convexity and monotonicity) of the problem to generate a deterministic sequence of points converging to an (local or global) optimal solution [74]. They are often represented through variations of NLP (continuous variables) and MINLP (integer and continuous variables) problem formulations, although there are also several other problem classes [75]. They provide insights regarding the local [74] or global optimality of a solution through analytical mathematical conditions [75]. From a practical perspective they require a lower number of objective function evaluations to reach an optimum solution than *stochastic* methods and enable the identification of locally [53] or globally [75] optimum solutions in non-convex problems. Limitations of these methods involve the computationally intensive use of derivative transformations and difficulties in the initialization of simulations when complex models are considered. A fundamental issue of deterministic methods is to transcend local optimality [74] hence the development of mechanisms to prevent the convergence in local optima in highly non-convex problems is also a very active research field [76].
- *Stochastic* optimization methods, *i.e.*, methods for which the outcome is random, are particularly suited for problems that possess no known structure that can be exploited. These methods generally require little or no additional assumptions on the optimization problem [74]. The three main classes of stochastic methods are: Two-phase methods, random search methods, and random function methods [74]. The most well-known representatives of stochastic methods are Genetic Algorithms and Simulated Annealing [52,53] which are also called metaheuristics. Simulated Annealing is a typical representative of random search methods which is easily implementable, robust and applicable to a very general class of global optimization problems [74]. Metaheuristics usually emulate physical systems in order to explore the solution space of a given problem and identify the optimum solution through a series of probabilistic transformations. These methods do not suffer from the same limitations as the deterministic methods because their inherent mathematical operations are simple, their algorithmic mechanisms provide venues to target the globally optimal domain and discrete design parameters are handled easier. They can even be applied to ill-structured problems for which no efficient local search procedures exist [74]. However, the lack of these limitations is traded-off for convergence to a distribution of nearly optimal solutions and sometimes for long computational times required for the implementation of the stochastic runs. These characteristics are not necessarily shortcomings as the distribution of nearly optimal scenarios provides statistical guarantees for the quality of the solutions. These methods are very useful at early design stages when there is a vast number of discrete or continuous decision options to be investigated. The existence of multiple close-to-target optimum solutions provides valuable design insights into the problem which can be reviewed and analyzed by users prior to transferring

meaningful conclusions onto a subsequent stage where the design problem can be defined with considerably less uncertainty.

Table 7. Merits and shortcomings of considered methods and objective functions in process optimization.

	Merits	Shortcomings
Deterministic methods	Fewer function evaluations than stochastic methods to reach an optimum, analytical mathematical determination of local or global optimum	Intensive computations, difficult simulation initialization in non-convex models, mechanisms to avoid local optima is an active research field, require knowledge of analytical problem properties (e.g., convexity, monotonicity)
Stochastic methods	Suitable for early stage design with extensive and discretized design spaces, easier to implement than deterministic methods, no knowledge of optimization problem structure is required, rich design insights from close but different optimum solutions	Larger number of function evaluations to identify optimum solution, statistical assessment of solution optimality
Single-objective formulations	Easy to implement, result in a single optimum solution	Need for well-defined problems, use of different objective functions results in different designs, an appropriate objective function needs to be selected
Multi-objective formulations	Handle multiple and often conflicting objectives simultaneously, results in a rich set of finite designs representing important trade-offs	More difficult to implement than single-objective formulation
Thermodynamic objectives	Useful for early design stages using less rigorous process models	Appropriate objectives need to be selected and combined, indirect and approximate association with costs
Economic objectives	Support detailed and realistic designs when used with sufficiently detailed process models	More complex objectives than cost or profit may be needed, appropriate objectives should be selected based on optimization formulations and goals

In the reviewed works the preference for global search algorithms based on meta-heurists such as Genetic Algorithms, Simulated Annealing or Particle Swarm Optimization over deterministic optimization algorithms is noticeable. Approaches based on deterministic global optimization techniques [75] remain yet to be implemented for ORC design problems. Among different software packages, the GAMS software (www.gams.com) includes several deterministic optimization solvers, while MATLAB (www.mathworks.com) includes both deterministic and stochastic solvers.

4.5. Single- vs. Multi-Objective Optimization and Types of Objective Functions

Another observation is the use of *multi-objective* optimization approaches which allows the simultaneous consideration of several different performance measures. *Multi-objective* optimization is important when the use of objective functions associated with economics involves high uncertainty (e.g., in cases of thermodynamic analysis or prior to sizing) and is often replaced by the simultaneous consideration of objectives such as exergetic and energetic efficiency. This method is also important when sustainability objectives need to be considered simultaneously with economics. Sustainability considerations are often in conflict with economics because they increase the associated costs. Such

trade-offs are unveiled using multi-objective optimization. Merits and shortcomings of such formulations as well as objective function types are summarized in Table 7.

In ORC design the choice of the objective function is very important. In some reviewed cases exergetic and thermal efficiency are used as design criteria but almost always together with some other index that is related with cost. From a thermodynamic perspective, two major and general objectives were mentioned in Section 4.3 as part of the work presented by Lecompte *et al.* [73] in terms of different ORC structures. In terms of economics, Novak Pintarič and Kravanja [77] mention that minimization of costs and maximization of profit are the most frequently used economic criteria in the design of industrial process systems. However, there are many other financial measures which can lead to different optimal solutions if applied in the objective function. Such measures involve the total annual cost (TAC), profit before taxes (PBT), payback time (PT), return on investment (ROI), net present value (NPV), internal rate of return (IRR) and equivalent annual cost (EAC). Novak Pintarič and Kravanja [78] extend their work to investigate the impact of using such criteria in *single-* and *multi-objective* optimization approaches. They break down the economic criteria into three classes: (a) Qualitative or non-monetary criteria (e.g., IRR or PT), (b) Quantitative or monetary criteria (e.g., Profit and TAC) and (c) Compromise criteria (e.g., NPV and TAC or Profit using depreciation with the annualization factor). The authors generally conclude that the NPV is the most appropriate objective function to use. Even so, sufficiently accurate process models are necessary so that the obtained results are both optimum and realistic.

- In *single-objective* optimization, they find that the Compromise criteria (NPV) are the most suitable because the obtained designs enable a fair compromise between profitability, operational efficiency, and environmental performance. The other criteria either favor solutions with small capital investment and cash flow but fast payback time and high profitability (Qualitative criteria) or vice versa (Quantitative criteria).
- In *multi-objective* optimization the NPV results in Pareto optimum designs that are close to the environmentally friendliest designs obtained by Quantitative criteria (e.g., Profit or TAC). On the other hand, the Qualitative criteria unveil environmental trade-offs in a much wider range.

5. Operation and Control of ORC Systems

5.1. Main Concepts and Computational Challenges

ORC systems operate in perpetually changing environments and therefore their operation should be constantly monitored and controlled. The main source of variation affecting the operation of ORC is the quality of the heat source. The heat source may experience changes in the flow rate and the temperature influencing the enthalpy content of the stream. Such changes would impact the degree of superheating in the outlet stream of the evaporator and the efficiency of the overall cycle. Other sources of variation in ORC are the efficiencies of the pump and the expander, and the heat transfer coefficients in the heat exchangers.

Feedback control is the main concept behind the maintenance of the controlled variables at predefined levels despite the influence of multiple and continuous disturbances. The key idea in feedback control is the utilization of the most recent information about the state of the plant through sensible and reliable measurements of the controlled variables. The controller actions are determined using the calculated deviation of the controlled variables from predefined set points (*i.e.*, reference points). The main

objective of process control remains the transfer of process variability from the most important in terms of profitability and product quality process streams and variables to process streams and variables of reduced importance. Such streams that are the recipients of the variability on valuable and therefore important variables are usually utility and auxiliary streams (e.g., air or water cooling streams, bypass streams, working fluid flowrate). For instance, in an ORC system variability in the heat source is transferred to the electric power generator which is attached to the expander. Electric power is usually intended to satisfy a critical specification on the power load. Therefore, variability in the power generation may be attenuated by the control system by manipulating the flow rate of the working fluid and/or the expander bypass stream. Obviously, either action would also affect the working fluid condensation and the cooling requirements in the condenser usually imposed by an air cooling system.

Feedback control operates in order to correct any deviations of the controlled variables from predefined set point levels after the effects of exogenous disturbances on the controlled variables has been sensed by the measurement sensors. The controller action is computed based on the calculated deviation from a pre-defined set point (*i.e.*, error in the controlled variables). Linear analysis of the outlined dynamic system with either Laplace transform or state space formulation are the most commonly used practices to analyze and investigate the process dynamics and interactions [79]. Overall plant dynamics include the dynamics of the associated process units such as heat exchangers, pumps, expanders and so forth, the implemented controllers, the incorporated actuators, and the installed sensors. The process representation by transfer functions through a Laplace transform of the governing differential equations enables the evaluation of the system dynamic characteristics. Alternatively, a state space representation enables the representation of multiple input, multiple output systems. Several controller design methods are available that aim to achieve the desired dynamic performance for the system [80].

Real time control applications are usually based on a control law that has been offline calculated. In this aspect, online calculations are limited to the evaluation of the control actions in a multi-loop fashion, where one manipulated variables is used to regulate one controlled variable, with minimal computational effort. This feature enables the implementation of a relatively small control interval; the time interval that a new control action is calculated and implemented in the system. However, such control systems must be designed with provisions to perform adequately even though the process has shifted away from the nominal operating point (e.g., due to a change in the power level) or process parameters have varied significantly during operation (e.g., due to fouling in the heat exchanger or other process equipment malfunctions). On the contrary, model-based control systems utilize at real time process model predictions that enable the controller to allocate the control effort in multi-variable systems optimally [81]. The achieved controller dynamic performance can be significantly improved over multi-loop approaches because input-output interactions are explicitly taken into consideration but at the expense of increased computational effort. Basically, dedicated control system can easily manage the involved computational effort, especially when the employed models are linear [82]. Nonlinear model predictive control systems [83] offer definitely improved accuracy of model predictions and therefore better control performance but require specialized solution algorithms for optimization and state estimation [84]. A schematic of the relationship between process detail involved in online control applications with the associated control effort is provided in Figure 6.

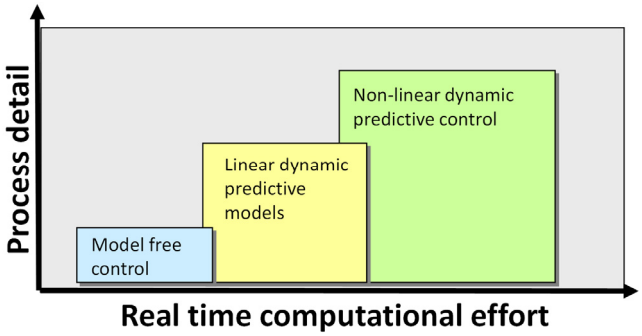

Figure 6. Control approaches with respect to process detail and real time computational effort.

5.2. Dynamic Models

Identifying the dynamics of ORC systems is important in the design and achieved performance of the control system. Process models that are based on first principles arising from the physical phenomena (e.g., heat transfer, compression, expansion) taking place in the ORC provide the most reliable and accurate description of the system behavior. The models are basically consisted of material, energy and momentum balances in dynamic mode accompanied with constitutive equations. However, the models involve a number of parameters associated with the physical and chemical phenomena (e.g., heat and mass transfer coefficients, expander and pump efficiencies, physical properties and so forth). The estimation of the model parameters requires the collection of experimental data from well-designed experiments with sufficiently rich information in calculating accurately the model parameters. The most reliable way for the parameter estimation is the fitting of the model response to the dynamic data using maximum likelihood principles and dynamic programming techniques. However, the development of a detailed mechanistic model can be replaced by empirical modeling performed using input-output data. This simplified technique requires the execution of experimental step changes in the input process variables while maintaining all other variables in manual operation [85]. The magnitude of the step change depends on the process nonlinearity and the measurement noise level in the measured variables. Depending on the shape of the output response of the process to an input step change, the order of the dynamic system can be identified. Most dynamic systems can be approximated as first-order models with dead-time [79]. Dead-time is the time it takes to observe the effect of an input signal change in the output variables. High order over-damped systems resemble the behavior of a first-order plus dead-time model and therefore it becomes an attractive modeling option. The estimation of the model parameters for such a model; namely the process gain, the time constant, and the dead-time, can be easily performed [86]. An alternative empirical model building is based on time series analysis [87]. Auto- and cross-correlation of time series can be utilized for the identification of the process model order whereas ordinary least squares and recursive least squares can be used for the estimation of the model parameters. Zhang *et al.* [88–90] have employed auto-regressive integrated moving average models in the control of ORC systems.

In a typical ORC system the main source of dynamic characteristics are the evaporator and the condenser. The evaporator is a heat exchanger with single phase (preheating and superheating) and double phase (evaporation) regions. Twomey *et al.* [91] developed a dynamic model for a solar ORC using a scroll expander. The dynamic model based on first principles showed good agreement with

experimental data regarding power output, rotational speed, and exhaust temperature. The effect of the tank volume which is being heated by the circulation of the solar collector fluid and is acting as the heat source for the system is investigated. The validated model is utilized in the design of solar thermal cogeneration systems that satisfies the peak power demand.

Wei *et al.* [92] attempted to capture the dynamics of the system heat exchangers using models based on moving boundary and discretization techniques. The moving horizon technique aims to identify the boundaries between a single (liquid or gas) and a two phase (gas and liquid) region within the evaporator by imposing explicit energy balances. In the discretization technique a number of computational cells is introduced within each region with the appropriate boundary conditions. The two methods are compared in terms of accuracy, complexity and simulation speed with the moving boundary technique exhibiting better characteristics for online control applications. However, the discretization methods appeared to be more suitable for the simulation of start-up and shut-down conditions.

Similarly, Bamgbopa and Uzgoren [93] developed a dynamic model for the heat exchangers and static models for the pump and the expander and studied the power output for varying flow rate and temperature for the hot and cold sources in a system that employed R245fa as the working fluid. In a subsequent article by Bamgbopa and Uzgoren [94] the models were utilized to evaluate the steady state efficiency of a solar ORC system. The values for the decision variables (hot source flow rate and temperature, and working fluid flow rate) that maximize the overall efficiency of the system were determined. Regression models were developed to characterize the effectiveness of the system in terms of the ratio of the working fluid flowrate to the heat source flow rate and the heat source temperature at the inlet of the evaporator. Table 8 summarizes the employed modeling approaches and the purpose of the developed model.

Table 8. Dynamic modeling approaches.

Authors	Modeling Method	Equipment	Purpose
Quoilin *et al.* [85]	Empirical (regression)	Entire ORC system	Control system design
Zhang *et al.* [88–90]	Empirical (regression)	Entire ORC system	Control system design
Wei *et al.* [92]	First principles	Entire ORC system	Start-up and shut-down simulations
Bamgbopa and Uzgoren [93]	First principles	Heat exchangers (dynamic), pump expander (static)	Power output computation
Bamgbopa and Uzgoren [94]	First principles	Solar ORC	Steady state efficiency

5.3. Control Approaches

Control systems for ORC can be generally categorized in multi-loop and multi-variable schemes. Quoilin *et al.* [95] proposed a series of control strategies for an ORC. Initially, a static model was used to determine the optimal evaporating temperature and superheating for a wide range of heat source and heat sink conditions. The manipulated variables in the system included the expander speed and the pump capacity. The optimal evaporator temperature was derived from a regression model and was followed by the control system consisted of two proportional-integral controllers. In another version of the control scheme a correlation was utilized for the pump capacity based on expander speed of rotation and the

heat and cool source temperature. This acts as a feedforward control system as the measurement of the expander speed was used to provide the set point for the working fluid flow rate. In this way the response of the control system was significantly faster. However, proper tuning of the controllers should be maintained in order to achieve stability. Simulated results verified that the control scheme that follows the optimal evaporation temperature trajectory exhibited superior performance. Peralez *et al.* [96] used a model based control scheme considering system inversion for the control of the superheating temperature which affects both cycle performance and system safety. The model inversion introduces a feedforward action in addition to the feedback controller to effectively compensate for disturbances in the evaporator. Kosmadakis *et al.* [97] discussed potential control strategies for double stage expanders in ORC systems.

Multivariable control schemes have attracted the attention of researchers in the control of ORC systems because of the superior performance they exhibit in ORC applications [98]. Zhang *et al.* [88] developed a dynamic model with moving boundaries for the evaporator and the condenser. Subsequently, a linear state space model was derived for control system design purposes. The control objectives were the minimization of system interaction in order to achieve good disturbance rejection and the maximization of the overall system efficiency. For the latter, the degree of superheating in the evaporator and the condenser outlet temperatures were regulated. A linear quadratic regulator coupled with a PI (proportional-integral) controller have been designed and simulated for set point changes in the power output and the throttle valve pressure (*i.e.*, pressure at the entrance of the expander) as well as the superheating and condenser temperatures. The PI controller maintained the condenser outlet temperature at the desired level. Similarly, disturbance rejection scenarios were investigated associated with hot gas stream velocity variation and throttle valve dynamics. Zhang *et al.* [99] extended the previous work by developing an extended observer that aims to provide accurate state estimates for the system.

Zhang *et al.* [89] introduced a dynamic model for a waste heat recovery system based on ORC with R245fa as the working fluid. The first principles dynamic model was then converted to a CARIMA (controlled auto-regressive integrated moving average) model for use in a model predictive control scheme. The controlled variables in the multi variable control scheme were the system power output, the evaporator pressure, the superheating temperature, and the condenser temperature. These variables were controlled using the pump and expander rotating speeds and the air flow in the condenser. A constrained generalized predictive controller [100] was implemented which rejected disturbances and followed set point effectively. In a subsequent paper, Zhang *et al.* [90] introduced a constrained generalized predictive controller that considered bounds on both the manipulated and controlled variables as well as the rate of change for the manipulated variables. The performance of the controller has been evaluated for disturbances in the temperature and the flow rate of the heat source stream. Power output was maintained at the desired level despite the disturbances. Additionally, set point changes for the evaporator pressure, the superheating temperature and the condenser temperature were successfully tracked by the controller.

In a recent work Hou *et al.* [101] introduced a minimum variance controller with real-time parameter estimation for a CARMA (controlled auto-regressive moving average) model. A recursive least squares technique was implemented for the parameter estimation. However, the proposed control scheme does not consider a model for the stochastic disturbances in the system. Uncertainties may play a significant role in the performance of the ORC system. Therefore, changes in the dynamic features should be monitored on-line using the measurements from the process. Additionally, the inherent nonlinearities in the system may make the predictions from linearized process models highly inaccurate. To this end,

Zhang *et al.* [88] proposed a state extended observer for the on-line update of states and model parameters. The updated model is then utilized in a linear quadratic regulator with a PI controller for the plant control.

Table 9 summarizes the literature in control strategies of ORC systems. In conclusion, multi-loop control systems works efficiently when good conceptual and process knowledge is utilized based on prior system analysis. Multi-loop control systems are easily implemented and maintained but may require frequent tune-up to account for process changes and operating condition variations. Multi-variable control systems require the development of a dynamic process model that can provide accurate process behavior predictions over a wide range of operation conditions. The implementation is definitely more challenging but guarantees good control performance through the explicit consideration of process interactions.

Table 9. Control approaches.

Authors	System Type	Control Approach	Manipulated/Controlled Parameters
Quoilin *et al.* [95]	Low grade ORC waste heat recovery	PID (multi-loop)	Pump speed, expander speed/evaporating temperature, superheating
Peralez *et al.* [96]	ORC waste heat recovery	Nonlinear model inversion	Exhaust gas by-pass valve, expander by-pass valve, pump speed, expander speed/Superheating temperature
Hou *et al.* [101]	ORC waste heat recovery	Minimum variance controller (multi-variable)	Throttle valve position, mass flow rate of working fluid, mass flow rate of exhaust gas, air flow rate/power, throttle pressure, evaporator outlet temperature, condenser outlet temperature
Zhang *et al.* [88,99]	ORC waste heat recovery	Linear Quadratic Regulator with extended observer (multi-variable)	Throttle valve position, working fluid pump speed, exhaust gas velocity, air velocity/power, throttle pressure, evaporator outlet temperature, condenser outlet temperature
Zhang *et al.* [89]	ORC waste heat recovery	Model predictive control (multi-variable)	Throttle valve position, working fluid pump speed, exhaust gas velocity, air velocity/power, throttle pressure, evaporator outlet temperature, condenser outlet temperature
Zhang *et al.* [90]	ORC waste heat recovery	Constrained generalized predictive controller (multi-variable)	Throttle valve position, working fluid pump speed, exhaust gas velocity, air velocity/power, throttle pressure, evaporator outlet temperature, condenser outlet temperature, Constraints on system variables.

Part load operation away of the nominal design ORC settings is an important issue that requires the utilization of efficient control methods. The operation of the ORC system at part load conditions also requires the modeling of the thermal efficiency with respect to the off-design operating conditions. We review some part load system analyses here however all works do not consider feedback control system performance but rather focus on steady state operation.

Ibarra *et al.* [102] focused on the characterization of the expander and the heat recuperator to obtain an accurate representation of the optimal part load conditions. The study involved a number of different working fluids. Manente *et al.* [103] provided correction factors for the turbine isentropic efficiency due to variations of the isentropic enthalpy drop and the working fluid mass flow rate from the design point. In this way the calculation of the sensitivity of performance indicators with respect to the off-design point was possible. The control system utilized subsequently the optimal operation point at part load. A cascade type of control has been implemented in the combined gas turbine—ORC system by de Escalona *et al.* [104]. The study focused on the benefits from the addition of the ORC for waste heat recovery and considered part load conditions in the ORC performance. Additional latest works and applications are reviewed in a recent work addressing the part load performance of a wet indirectly fired gas turbine integrated with an ORC turbogenerator [105].

5.4. Remarks on Employed Methods

Control of ORC systems enables the efficient compensation of the effect disturbances have on the power output and guarantee the equipment operation within safety limits.

- Multi-loop control systems are relatively simple to implement but require careful tuning to enable stable and acceptable dynamic performance. Highly interactive systems hinder the achievable control performance and therefore the introduction of model based control techniques becomes a viable option. System interaction is further increased whith more complex ORC configurations (e.g., multi-pressure or multi-temperature systems, multiple expansion units and so forth).
- Model based control systems require the development of accurate dynamic models for the individual subsystems. Usually, linear models with suitable disturbance models and integral action can meet the control objectives. The model development effort is accompanied by the execution of well-designed experiments in order to estimate model parameters and validate the model structure and predictions. In addition, an online parameter estimation procedure is attached to the feedback loop so that the control models can adapt to plant drifts. Model based control usually results in improved dynamic performance as process interaction is taken into consideration explicitly but model accuracy is an essential factor for acceptable set-point tracking and disturbance rejection.

6. ORC Integration with Multiple Heat Source Streams

6.1. Main Concepts

The work reviewed so far has focused on working fluid selection, ORC design optimization and control with respect to a single heat source and sink. Energy intensive industrial processes often require significant amounts of low to medium grade heat to be removed into cooling water or another cooling medium, which could be utilized through synergies with surrounding processes and sectors [106]. ORCs offer a potentially promising route to monetize this waste heat through conversion to power. Besides the widespread industrial processes, other applications with multiple heat sources have been identified. Romeo *et al.* [107] integrate the multiple intercoolers in compression trains with ORC configurations. The work designs the cycles (high and low pressure) together with the compression train to match

intercooling waste heats and the ORCs. The work demonstrates significant energy savings of over 10% from the integration on the ORCs with the compression train. In another application, Soffiato *et al.* [108] integrate ORCs with the available waste heat streams onboard a LNG carrier. The work shows that power output can be increased by 3.5% through ORC integration. DiGenova *et al.* [2] study the integration of ORCs with an energy intensive Fischer-Tropsch plant to convert coal to liquid fuels. They apply the Pinch Analysis techniques to explore the performance of single and multi-pressure cycles to convert heat from process streams to power and observe that the carefully integrated ORCs significantly outperform steam cycles in terms of conversion efficiency.

Although systematic approaches for the integration of ORC systems with multiple heat source streams are only emerging, the general field of process energy integration, in which most proposed approaches have their roots, is well established. In the 1970s, energy integration approaches emerged with the advent of Pinch Analysis for targeting minimum process heat requirements and heat recovery network design [109]. The methods are well established and routinely applied in the design of chemical processes [110], which has led to significant energy savings in the process industries. These approaches have their origin in thermodynamic analysis and provide graphical representations of the design problem to guide the analysis of energy flows and gain insights into promising heat recovery and power generation options [111]. To enable the better screening of design options and to incorporate economic criteria in decision making, numerous complementary approaches based on mathematical optimization have emerged over time to explore both operational design decisions as well as structural design alternatives for process heat and power systems. Smith [110] provides an overview of established energy integration approaches. The graphical approaches do not present computational challenges, whereas the optimization-based process integration approaches incorporate similar challenges to those reported in Section 4.

6.2. Reviewed Approaches

The integration of ORCs with multiple heat source streams and in the context of process heat and power generation systems has had no reference in the literature until very recently. Over the past five years, systematic approaches to guide the efficient integration of ORC systems have started to emerge (Tables 10 and 11). Hackl and Harvey [112] employ Total Site Analysis for power production from low temperature excess process heat from a chemical cluster using a simple ORC. Desai and Bandyopadhyay [113] were the first to study the integration of ORCs with a background process of multiple potential heat source streams. They adopt graphical approaches and apply established Pinch analysis techniques in the form of Grand Composite Curves to explore ORC integration targets and develop heat exchanger network designs to achieve them. The work highlights the strong dependence of high performance ORC integration strategies on the specific characteristics of the background process. With a focus on site utility systems with multiple steam levels and turbines, Kapil *et al.* [114] introduce a co-generation targeting method that considers the optimization of pressure levels together with integration options for ORCs and heat pumps as low grade heat utilization options.

Hipolito-Valencia *et al.* [115] propose a superstructure approach to capture various possible heat transfer options between process streams and the ORC. Similar to the work by Desai and Bandyopadhyay [113], the approach focusses on the efficient integration of the ORC with the multiple source streams of the background process. In a subsequent contribution, Hipolito-Valencia [116] propose

an approach for interplant energy integration that considers ORCs for power generation. Lira-Barragán *et al.* [117] continue this approach to select the best possible conditions, heat exchanger network configuration and type of process in a trigeneration system. The process types involve a steam Rankine cycle, an ORC and an absorption refrigeration system. The authors consider economic, environmental and social indices as objective functions in optimization. All three works resulted in MINLP formulations that were searched using deterministic optimization solvers. Neither approach optimizes the expansion section of the ORC.

Gutiérrez-Arriaga *et al.* [118] proposed an approach for energy integration involving waste heat recovery through an ORC which is based on a two-stage procedure. In the first stage, heating and cooling targets are determined through heat integration. This enables the identification of the excess process heat available for use in the ORC. The optimization of the operating conditions and design of the cogeneration system are carried out in the second stage using Genetic Algorithms.

Table 10. Optimization-based heat source integration approaches.

Authors	Integration Approach	Evaluated Options	Integration/Design Criteria
Kwak *et al.* [119]	Total site analysis, optimization of ORC operation	Sixteen working fluids, turbine inlet temperature condenser outlet temperature	Total annualized cost
Chen *et al.* [120]	Superstructure-based optimization of HEN integrated with ORC, MINLP solver	Number and connections of HEN, operating parameters of HEN and ORC	Generated ORC work
Marechal and Kalitventzeff [121]	Mathematical model of exergy composite curves (MILP solver), ORC operation optimization and fluid selection (MILP solver)	List of few pre-selected fluids, utility flowrates, several ORC operating characteristics	Costs, exergy losses
Soffiato *et al.* [108]	SQP solver (deterministic) for ORC optimization in an iterative procedure, pinch composite curves for ORC-heat source matching, evaluation of each ORC structure and working fluid combination	Six working fluids, three pre-selected structures (simple cycle, regenerative cycle, and two-stage cycle), the evaporation pressures and the degrees of superheating in one or two stages, the ratio between the mass flow rates in the two stages	Net ORC power output
Lira-Barragán *et al.* [117]	Multi-objective MINLP, results reported for all working fluids	Three working fluids, structure and operating characteristics of heat exchanger network, existence of ORC and/or absorption refrigeration system	Economic (annual profit), environmental (greenhouse gas emissions), social (number of jobs generated)
Gutiérrez-Arriaga *et al.* [118]	Pinch grand composite curves, Genetic Algorithms to optimize operation of a basic ORC, results reported for 3 different working fluids	Three working fluids, operating ORC parameters	Gross annual profit
Kapil *et al.* [114]	Total site analysis (NLP optimization), ORC process simulation	Pressure of different steam levels	Enthalpy difference of shifted heat sink and source, thermal efficiency, purchase cost
Hipólito-Valencia [115,116]	Heat exchanger network superstructure, MINLP solver	Total heat transfer area, network configuration, operating parameters, two working fluids	Total annualized cost

Kwak *et al.* [119] investigate different technologies, including ORCs for energy recovery and exploitation in different industrial sites. The authors perform a Total Site Analysis to identify energy recovery targets and then identify the optimum ORC operating parameters together with the working fluid (from a list of 16 pre-defined fluids) in order to best recover the available energy.

Chen *et al.* [120] present a mathematical model for the synthesis of a heat-exchanger network (HEN) which is integrated with an organic ORC for the recovery of low-grade industrial waste heat. An ORC-incorporated stage wise superstructure considering all possible heat-exchange matches between process hot/cold streams and the ORC is first presented. First, a stand-alone HEN is synthesized to minimize the external utility consumption. An ORC is then incorporated into the HEN with the objective of maximizing the work produced from waste heat (without increasing the use of a hot utility. The problem is formulated and solved as a two stage MINLP.

Marechal and Kalitventzeff [121] proposed a method for the investigation of ORC process characteristics which is based on the analysis of the shape of the grand composite curve, combined with the use of the minimum exergy losses concept, heuristic rules and a cost optimisation technique. First, the recovery targets of the background (waste-heat) industrial process are determined through an MILP-based optimization to minimize exergy losses using the utility flowrates as decision variables. ORCs are then designed together with working fluids selected from a pre-specified list to optimally match the identified energy recovery opportunities. The identified ORCs are characterized in terms of the condenser and evaporator temperatures and pressure conditions, the opportunity for superheating, the expected flow-rate and efficiency of the cycle. The non-linear cost estimation of the condensers, boilers, turbines and pumps are linearized and the best matches of the designed ORCs with the background process are identified using MILP-based optimization to minimize costs. The focus of the proposed developments is on the integration of the ORC vaporization and condensation sections.

Stijepovic *et al.* [70] adopt the exergy composite curves (ECCs) approach developed by Linnhoff and Dhole [71] to explore the potential for ORC process improvements through better utilization of the available heat. The ECC shape reflects on ORC operating conditions which may be interpreted by different process configurations (e.g., simultaneous consideration of different pressure levels may require multiple turbines interconnected at various heat exchanger topologies to match the necessary temperatures). Details of this approach have been reviewed in Table 6.

Most recently, Song *et al.* [122] explores integration schemes for single and dual ORCs with multiple waste heat streams through simulation. The work identifies the dual cycle as the best performing configuration for a refinery case study. This highlights the need to develop optimal ORC integration methods in the future that can take into account multiple heat source streams and multiple integrated power cycles simultaneously.

Tchanche *et al.* [123] developed an approach to evaluate the performance of different ORC configurations by using several criteria based on exergies for different parts of the equipment. Using graph theory they conceptualized the exergy flows and losses within different sections of an ORC system, investigating three different cycle topologies in the condensing and pumping sections (*i.e.*, regenerative heat exchanger, open feed liquid heater and closed feed liquid heater).

Yu *et al.* [124] propose a new method to simultaneously determine the working fluid and operating conditions in an ORC. The Preheating Pinch Point and the Vaporization Pinch Point are introduced. The method is based on a newly defined parameter named “predictor” that can predict the pinch position

between the waste heat carrier and the working fluid, calculate the mass flow rate of working fluid and the amount of heat recovered, and determine the optimum working fluid and corresponding operating conditions simultaneously. The authors consider 11 pre-selected working fluids which are considered as decision options simultaneously with the process features. The objective is to maximize the power output without considering the equipment cost and operating expenses.

Safarian and Aramoun [125] employ a combined energy- and exergy-based analysis approach to evaluate four ORC configurations, namely a basic ORC, an ORC with turbine bleeding, with regeneration and with both turbine bleeding and regeneration. The authors employ several analysis criteria, calculate exergy losses and find that the evaporator has major contribution in the exergy destruction which is improved by increase in its pressure. Furthermore, the configuration with turbine bleeding and regeneration enables a maximization of thermal and exergetic efficiencies and minimization of exergy losses.

Luo *et al.* [126] present s systematic hybrid methodology of graphical targeting and mathematical modeling to address the optimum integration of a regenerative ORC in a steam network. The objective function is to minimize the fuel consumption of the steam power plant. The terminal temperature and heat load of the process-heated boiler feed water are the two decision variables. The graphical targeting method is proposed to ascertain the bounds and constraints of the two decision variables. A mathematical model incorporating rigorous simulations of the turbine is formulated to achieve the optimal heat integration scheme.

Table 11. Graphical or simulation-based heat source integration approaches.

Authors	Integration Approach	Evaluated Options	Integration/Design Criteria
Yu *et al.* [124]	Pinch-based energy recovery targeting, iterative enumeration	Eleven working fluids, cycle operating parameters	Power output
Safarian and Aramoun [125]	Exergy- and energy-based analysis to identify best ORC structure, evaluation of each structure separately	Basic ORC, ORC incorporating turbine bleeding, regenerative ORC, ORC incorporating both turbine bleeding and regeneration	Degree of thermodynamic perfection, exergetic efficiency, thermal efficiency, influence coefficient, exergy loss
Luo *et al.* [126]	Pinch-based energy targeting, simulation-based objective function evaluation	Terminal temperature and heat load of the process-heated boiler feed water	Fuel consumption of steam power plant
Tchanche *et al.* [123]	Energy and exergy flow analysis, evaluation of each working fluid and ORC structure combination separately through simulations	Four working fluids, four structures (basic ORC, ORC with regenerative heat exchanger, with open or closed feed liquid heater)	Exergy losses, degree of thermodynamic perfection, exergetic efficiency, energetic efficiency
Romeo *et al.* [107]	Pinch-based energy integration, different temperature levels, evaluation of ORC structure for each working fluid	Pre-selected two-stage (dual pressure) ORC, temperature of waste heat source, six pre-selected working fluids	Energetic efficiency
DiGenova *et al.* [2]	Pinch composite curves for ORC-heat source matching options, evaluation of each structure separately	Five ORC structures (basic ORC, with reheat stages, with multiple pressure levels, recuperator and balanced recuperator)	Thermal efficiency

Table 11. *Cont.*

Authors	Integration Approach	Evaluated Options	Integration/Design Criteria
Hackl and Harvey [112]	Total site analysis, ORC simulations with different working fluids	Five pure fluids, one mixture, ORC operating parameters	Net excess heat, cost of electricity, payback period of investment, CO_2 emissions reduction
Desai and Bandyopadhyay [113]	Pinch-based graphical integration, ORC simulations with different fluids	Sixteen fluids, basic ORC, ORC with turbine bleeding and regeneration, heat exchanger network configuration and conditions	Net work output, thermal efficiency
Song *et al.* [122]	Matching of heat sources at different temperatures with different ORC configurations and fluids, simulations	Eight pure and six mixed working fluids, Dual integrated or independent ORC, single ORC	Net power output, heat transfer area and their ratio

6.3. Remarks on Integration

Despite the recent progress, there remains significant scope to develop more widely applicable, systematic approaches to guide the optimal integration of ORCs with multiple heat streams in the context of background processes. Future developments are expected to focus on a number of unexplored aspects of the ORC integration problem:

- Enriched representations of ORC configurations and multiple heat steams in the form of superstructures to provide a representation of all possible alternative configurations, including multi-pressure and multi-cycle systems.
- Multi-scale approaches to bridge the gap between higher-level ORC integration and detailed design decisions impacting on performance such as heat exchanger design optimization.
- Multi-scale approaches to support integrated decision making across the working fluid selection, ORC design and ORC integration problem levels, and
- Global search schemes for ORC integration with multiple heat sources similar to the approaches that emerge for ORC design optimization.

An important observation is that most existing works consider energy analysis, although the combination of energy and exergy analysis is also very useful for the investigation of different ORC configurations and integration options. Usually, energy analysis takes into account only wasted heat which is available at temperatures where it may be re-utilized as heat (e.g., steam). However, wasted heat of low enthalpy content may be transformed into power through ORC and re-utilized in the process. Exergy analysis is particularly relevant in these cases as it focuses on the maximum useful work that can be produced from a heat source. When heat is transferred part of the thermal energy is degraded due to process irreversibility. The key is to minimize the part of thermal energy lost due to degradation. Exergy is the maximum quantity of work that can be produced in a cyclic thermodynamic process. It captures only that part of the thermal energy which may be transformed into work. Energetic analysis targets the recovery of heat loads. Exergetic analysis targets the maximum work that may be recovered from an available heat source, hence it may target exergy loss or the ideal work equivalent lost in heat transfer.

7. Concluding Remarks

The design of ORC systems is a challenging task. Many design alternatives exist at each level of design, from working fluid selection via cycle optimization and control through to the efficient integration of the cycle with background processes. A number of systematic approaches have emerged over the past few years that aim at supporting the designer in making optimal choices at each level of ORC development. This paper has aimed to provide a state-of-the-art overview of these emerging approaches with a particular emphasis on computer-aided design methods and aimed to highlight areas that may benefit from further research and development.

Author Contributions

The three authors jointly developed this review article. Individual focus areas have been computer-aided ORC working fluid design and selection (A.I. Papadopoulos), ORC design and integration (P.Linke) and ORC operation and control (P. Seferlis).

Nomenclature

CAMD	Computer-Aided Molecular Design
CARMA	Controlled auto-regressive moving average
CFD	Computational fluid dynamic
CoMT	Continuous molecular targeting
COSMO-RS	Conductor-like screening model for real solvents
DFT	Density functional theory
EAC	Equivalent annual cost
EoS	Equation of state
GC	Group contribution
GWP	Global warming potential
HEN	Heat exchanger network
IRR	Internal rate of return
MILP	Mixed integer linear programming
MNLP	Mixed integer non-linear programming
NLP	Non-linear programming
NPV	Net present value
ODP	Ozone depletion potential
ORC	Organic Rankine cycle
PBT	Profit before taxes
PC-SAFT	Perturbed chain statistical associating fluid theory
PI	Proportional-integral
PID	Proportional-integral-derivative
PT	Payback time
QSPR	Quantitative structure-property relationships
ROI	Return on investment
SQP	Sequential quadratic programming
TAC	Total annual cost

Conflicts of Interest

The authors declare no conflict of interest.

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