Applied Thermal Engineering 90 (2015) 64–74

Contents lists available at ScienceDirect

Applied Thermal Engineering

journal homepage: www.elsevier.com/locate/apthermeng

Research paper

Parametric investigation of working fluids for organic Rankine cycle applications

J. Steven Brown*, Riccardo Brignoli, Timothy Quine

Department of Mechanical Engineering, Catholic University of America, Washington, DC 20064, USA

HIGHLIGHTS

- "Ideal" working fluids are investigated for organic Rankine cycles (ORC).
- The thermodynamic space of "ideal" working fluids is parametrically investigated.
- Five low- and high-temperature ORC applications are investigated.
- 1620 "ideal" and several "real" working fluids per application are investigated.

ARTICLE INFO

Article history:
Received 27 March 2015
Accepted 21 June 2015
Available online 9 July 2015

Keywords:
Equation of state
Organic Rankine cycle
Parametric study
Peng-Robinson
Working fluids

ABSTRACT

This paper investigates working fluids for organic Rankine cycle (ORC) applications with a goal of identifying "ideal" working fluids for five renewable/alternative energy sources. It employs a methodology for screening and comparing with good engineering accuracy the thermodynamic performance potential of ORC operating with working fluids that are not well characterized experimentally or by high-accuracy equations of state. A wide range of "theoretical" working fluids are investigated with the goals to identify potential alternative working fluids and to guide future research and development efforts of working fluids. The "theoretical" working fluids investigated are described in terms of critical state properties, acentric factor, and ideal gas specific heat capacity at constant pressure and are obtained by parametrically varying each of these parameters. The performances of these "theoretical" working fluids are compared to the performances of several "real" working fluids. The study suggests a working fluid's critical temperature and its critical ideal gas molar heat capacity have the largest impact on the cycle efficiency and volumetric work output, with "ideal" working fluids for high efficiency possessing critical temperatures on the order of 100%–150% of the source temperature and possessing intermediate values of critical ideal gas molar heat capacity.

1. Introduction

Organic Rankine cycles (ORC) produce electricity from low-temperature, non-traditional energy sources such as geothermal, biomass, waste heat recovery, and solar, with each representing 73%, 14%, 13%, and 0.5%, respectively, of current ORC applications [1]. Ref. [1] estimates the total worldwide installed electricity capacity of ORC in 2011 was 1.3 GW and [2] estimates the total worldwide installed electricity capacity for all energy sources in 2011 was 5331 GW. Thus, ORC represents a very small fraction of the total, namely, only 0.024%. Therefore, wider application of ORC could improve energy sustainability by increasing the mix of renewables and alternative energy sources in the production of electricity.

One obstacle—among others—inhibiting wider spread use of ORC is that each application is essentially unique with different capacity, energy source and its temperature, low-temperature sink and its temperature, system components, and working fluid, to name a few. The latter is the focus of the current paper. While there is no claim here to review the literature, the interested reader is referred to a few recent papers [3–17] which focus primarily on working fluids for ORC applications. Bao and Zhao [3] reviewed a large number of literature sources and identified 77 commonly

* Corresponding author. Department of Mechanical Engineering, Catholic University of America, 620 Michigan Ave, NE, Washington, DC 20064 USA. Tel.: +1 202 319 5170; fax: +1 202 319 5173.
E-mail addresses: brownjs@cua.edu (J.S. Brown), r.brignoli@outlook.com (R. Brignoli), 18quine@gmail.com (T. Quine).

http://dx.doi.org/10.1016/j.applthermaleng.2015.06.079
1359-4311/

Nomenclature

c_p^o	ideal gas specific heat at constant pressure [kJ/kg·K, kJ/kmol·K]
h	specific enthalpy [kJ/kg]
$\dot{m}$	mass flow rate [kg/s]
P	pressure (kPa)
R	universal ideal gas constant [kJ/kmol·K]
$\dot{Q}$	heat transfer rate [kW]
T	temperature [°C, K]
T^*	non-dimensional temperature, $T^* = T_r = T/T_c$
s	entropy [kJ/kg K]
s^*	non-dimensional entropy $= (s - s_{f,T_r=0.7})/s_{fg,T_r=0.7}$
v	specific volume [m^3/kg]
V	volumetric work output [kJ/m^3]
$\dot{W}$	power [kW]
x	quality
Z	compressibility factor

Greek symbols

η_{IHX}	internal heat exchanger effectiveness [%]
η_p	pump isentropic efficiency [%]
η_t	turbine isentropic efficiency [%]
η	cycle thermal efficiency [%]
Π	integral of c_p^o over the temperature range $0.7 \le T_r \le 1.0$, $= \int_{0.7T_c}^{1.0T_c} c_p^o \cdot dT$, see Eq. (5)
ρ	density [kg/m^3]
ω	acentric factor

Subscripts

0,…,10	thermodynamic state points (Fig. 1)
boil	boiler
c	critical
Carnot	Carnot
cond	condenser
est	estimated
f	saturated liquid
fg	difference between saturated vapor and saturated liquid
g	saturated vapor
−IHX	without internal heat exchanger
+IHX	with internal heat exchanger
max	maximum
p	pump
r	reduced
ref	reference
sat	saturation
source	source
t	turbine

Acronyms

EoS	equation of state
GWP	global warming potential
HCFC	hydrochlorofluorocarbon
HFC	hydrofluorocarbon
IHX	internal heat exchanger
NBP	normal boiling point
ODP	ozone depletion potential
ORC	organic Rankine cycle
P-R	Peng-Robinson
WHR	waste heat recovery

existing single-component working fluids and 44 zeotropic blends appearing in the various papers they reviewed. The identified working fluids are all well-described ones, that is, they are ones that are well-characterized by considerable experimental data and/or they are ones for which high accuracy Equations of State (EoS) are available. Brown et al. [4] proposed a methodology for estimating thermodynamic parameters and performance of working fluids for ORC using the Peng-Robinson (P-R) EoS and demonstrated this approach to be simple and sufficiently accurate – for engineering calculations – for evaluating ORC performance for both well-described working fluids and for not-so-well-described working fluids (little or no experimental data and/or high-accuracy EoS are available). Brignoli and Brown [5] extended the methodology of [4] and developed a simulation model capable of modeling well-described and not-so-well-described working fluids in ORC applications. Lai et al. [6] investigated 13 potential working fluids described with BACKONE and PC-SAFT EoS for high-temperature ORC applications. Saleh et al. [7] investigated 31 potential working fluids described with BACKONE EoS for low-temperature ORC applications. Maizza and Maizza [8] considered 24 working fluids, including eight zeotropic blends and one azeotropic blend, for waste heat recovery ORC applications. Chen et al. [9] compared the performance potential of carbon dioxide in a transcritical power cycle with a subcritical ORC operating with R123 for waste heat recovery applications. Drescher and Brüggemann [10] identified the family of alkylbenzenes as yielding the highest thermal efficiencies for biomass-powered ORC operating at 573 K. Lakew and Bolland [11] investigated six working fluids for low-temperature ORC applications and identified R227ea as yielding the highest power output among the six. Several papers [12–17] employ molecular design and optimization methodologies to choose/design an optimal working fluid and thermodynamic cycle for low-temperature ORC applications. In particular, Papadopoulos et al. [12,13] systematically designed and selected working fluids by applying computer aided molecular design for single-component working fluids and binary blends, respectively. They used multi-objective optimization methods to identify optimal working fluids subject particularly to criteria based on flammability, toxicity, ozone depletion potential (ODP), and global warming potential (GWP). Lampe et al. [14,15] simultaneously optimized the working fluid and thermodynamic cycle using the PC-SAFT equation of state. They mapped PC-SAFT parameters to real working fluids and interrogated a database of 200 working fluids. Palma-Flores et al. [16] coupled optimization techniques and computer aided molecular design to create a new family of organic working fluids and Molina-Thierry [17] simultaneously optimized blends of working fluids and the thermodynamic cycle for low-temperature ORC applications.

The current paper extends the methodology of [4,18] and uses the simulation model of [5] to investigate a large number of theoretical working fluids which are described in terms of critical state properties, acentric factor, and ideal gas specific heat at constant pressure for five different ORC applications. To extend the methodology of Brown et al. [4] a new empirical correlation that allows for calculating the critical density as a function of the critical ideal gas specific heat is developed. For each application, we investigate