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Design and selection of working fluid for Rankine-based Carnot battery based on the group contribution method#

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ABSTRACT

Recently, Carnot batteries, as an emerging electrical energy storage technology, are expected to solve the renewable electrical energy storage challenges faced globally. The selection of the working fluid is crucial to improving the system performance; however, the selection of existing working fluids is limited to a predefined database, and this approach does not allow for the design and discovery of novel working fluids. Therefore, in this paper, a model-based group contribution method for cross-scale preferential selection of working fluids was proposed for Rankine-based Carnot batteries. The result shows that the absolute average relative deviation of power-to-power efficiency, coefficient of performance, and power generation efficiency are 8.5%, 5.9%, and 2.6%, respectively.

Keywords: Rankine-based Carnot battery, Group contribution method, Screening of working fluid

NONMENCLATURE

Abbreviations	
AARD	absolute average relative deviation
COP	coefficient of performance
GWP	global warming potential
LCOS	levelized cost of storage
ODP	ozone depletion potential
P2P	power-to-power efficiency
Symbols	
P_c	critical pressure (bar)
T_b	boiling temperature (K)
Tc	critical temperature (K)
ω	acentric factor
ρ	saturated liquid density (kg/m³)
η_{orc}	power generation efficiency

1. INTRODUCTION

As the global energy paradigm continues to accelerate its transformation, energy security will probably face more complex challenges. Renewable energy is being developed and utilized in large quantities in China to reduce energy consumption, reduce environmental pollution, and achieve the goal of sustainable development [1]. Based on this, innovative energy storage is increasingly becoming a key technology for building new energy systems and new power systems. Rankine-based Carnot battery, as a new type of electrical energy storage technology, is not limited by geographical conditions, has a long-life cycle as well as high energy storage density, and has received widespread attention [2].

The physical properties of the working fluid directly determine the cycling performance [3], as an indispensable carrier for the energy conversion of the Rankine-based Carnot battery energy storage system. Therefore, the selection of the working fluid is the key to the development of an efficient thermal cycle. At present, several studies have been conducted focusing on the selection of the working fluids based on Rankine Carnot batteries. Aditya et al. [4] screened 16 working fluids considering low global warming potential (GWP) and zero ozone depletion potential (ODP) requirements. Frate et al. [5] selected 17 working fluids from the Coolprop database, considering the flammability, toxicity, and GWP of the refrigerants, and finally identified R1233zd (E) as the best working fluid. Eppinger et al. [6] selected four commonly used organic working fluids (Cyclopentane, R365mfc, Novec 649, and R1233zd (E)) and investigated their performance. Fan et al. [7] analyzed the thermodynamic performance and

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economics of two Rankine Carnot cell systems with and without heat rejection in terms of work pairs, and the results showed that in the system with heat rejection, R245fa-HFO-1336mzz(Z) had the best economics with a minimum levelized cost of storage (LCOS) of 0. 263 $/kWh, while in the system without heat rejection, HFO-1336mzz(Z)-R245fa has the best thermodynamic performance with an efficiency of 19.88%. However, these working fluid preference methods have been largely based on predetermined databases, and this approach cannot be investigated or designed for working fluids that have not yet been developed.

Based on the above studies, this paper proposes a cross-scale preferred Rankine-based Carnot battery working fluid model based on the group contribution method. The model can realize the study of molecular structure-fundamental physical properties-system performance, to facilitate the subsequent realization of computer-aided design and development of new working fluids. This method can be used to subsequently guide the screening of the working fluid of the Rankine-based Carnot battery.

2. MODEL AND METHODOLOGY

The schematic diagram of a Rankine-based Carnot battery is shown in Fig.1. The system consists of three main subsystems: heat pump, thermal storage, and organic Rankine cycle. In heat pump mode, the organic working fluid absorbs heat from low temperatures, which is compressed by the compressor and flows into the condenser, where the high-temperature heat is taken away by the thermal storage medium and stored in a high-temperature storage tank. When peaking is required, the working fluid absorbs heat from the high-temperature storage tank in the evaporator through the organic Rankine cycle mode, driving the generator to generate electricity through the expansion of the expander, and then enters the condenser to release the waste heat, and finally pressurizes back into the evaporator through the working fluid pump.

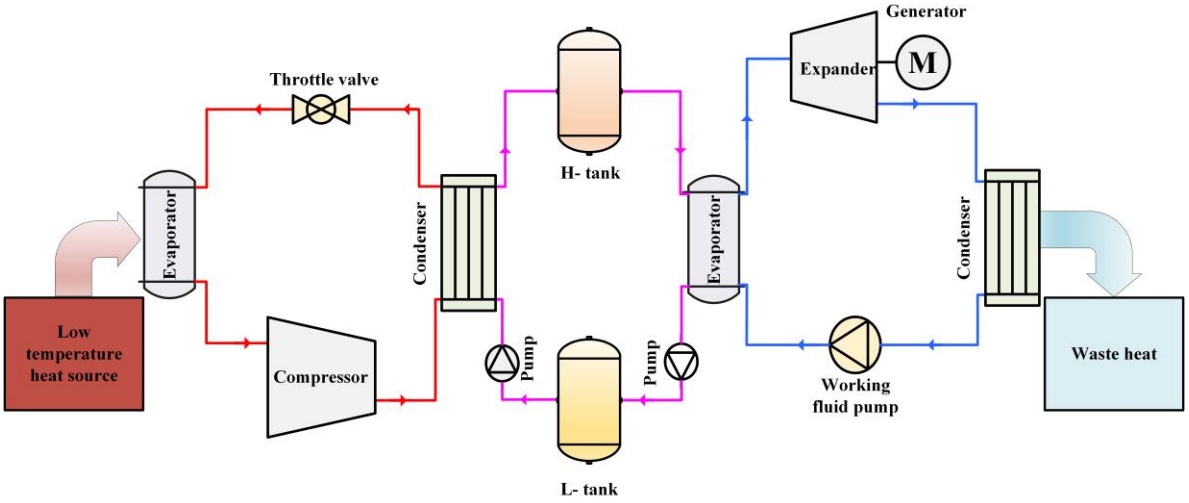

Fig. 1 The schematic diagram of a Rankine-based Carnot battery

2.1 Group contribution method model

Precise calculation of physical properties constants is a prerequisite for developing the optimization model of cross-scale organic working fluids for Rankine-based Carnot batteries. In this paper, the basic physical properties of organic working fluids are obtained by the group contribution method[8-10], and the steps are shown as follows:

1) The boiling temperature (T_b)

$$T_{\mathrm{b}} = 198.2 + \sum_k N_k t_{bk} \tag{1}$$

2) The critical temperature (T_c)

$$T_c = T_b / (0.584 + 0.965 \sum_k N_k t_{ck} - (\sum_k N_k t_{ck})^2) \tag{2}$$

3) The critical pressure (P_c)

$$P_c = (0.113 + 0.0032 \mathrm{n}_A - \sum_k N_k p_{ck})^2 \tag{3}$$

4) The acentric factor (ω)

$$\omega = \frac{0.3\left(0.2803 + 0.4789 T_{\mathrm{b}}/T_{\mathrm{c}}\right)\log P_c}{\left(1 - T_{\mathrm{b}}/T_{\mathrm{c}}\right)\left(0.9803 - 0.5211 T_{\mathrm{b}}/T_{\mathrm{c}}\right)} - 1 \tag{4}$$

5) The saturated liquid density (ρ)

$$\rho = \frac{M}{(17.5 + \sum_k N_k v_k)(0.29056 - 0.08775\omega)^{\beta}} \tag{5}$$

2.2 Thermodynamic cycle model

The power-to-power efficiency (P2P) is a key metric for the Rankine-based Carnot battery and can be calculated as follows:

$$P2P = \eta_{sto}\eta_{orc}COP \quad (6)$$

Where coefficient of performance (COP) and power generation efficiency (η_{orc}) are obtained through the coupling of fundamental thermophysical properties and thermal processes such as evaporation, condensation, compression, and expansion.

2.3 Boundary conditions

In this paper, a series of boundary conditions are shown in Table. 1 [11-13].

Table. 1 Boundary conditions

Parameter	Unit	Value
Mass flow rate of heating source (m_{hs})	kg/s	50
Heat source inlet temperature (T_{hs1})	℃	80
Thermal storage temperature (T_{up})	℃	90
Cooling water inlet temperature (T_{cw1})	℃	20
Pinch point temperature difference (ΔT_{pp})	℃	5
Heat storage efficiency (η_{sto})	-	0.95
Isentropic efficiency of compressor (η_{com})	-	0.85
Isentropic efficiency of expander (η_{exp})	-	0.8
Isentropic efficiency of pump (η_{pum})	-	0.8

3. RESULTS AND DISCUSSION

In this section, the basic physical properties (boiling temperature, critical properties, acentric factor, saturated liquid density) of 21 organic working fluids commonly used in thermodynamic cycling and the whole system performance (power-to-power efficiency, coefficient of performance, power generation efficiency) of the different working fluids are analyzed and discussed for estimating the precision of the developed cross-scale model.

3.1 Analysis of the basic physical properties

The basic physical properties of the twenty-one organic working fluids (in Table. 2) and Fig. 2 shows the relative error distribution of the basic physical properties predicted by Joback et al. based on the group contribution method.

In Fig. 2, the absolute value of the relative error of the boiling temperature is almost in the range of 10%; only the absolute value of the relative error of R245fa, R290, and R600a is higher than 10%. The absolute average relative deviation (AARD) for the boiling temperature is 5.91%. The prediction of the critical temperature is closely related to the boiling temperature and the group contribution to the critical temperature, according to Eq. (2). When the predicted boiling temperature is shorter than the actual boiling temperature, the predicted critical temperature is also lower than the actual critical temperature. Consequently, the AARD of the critical temperature is higher than the AARD of the boiling point temperature, which is 6.25%. Therefore, the high-accuracy prediction of the boiling temperature is one of the keys to ensuring the precision of the critical temperature prediction.

For critical pressure, the AARD is 6.47%, and the relative errors of the 16 organic working fluids are in the range of -10% to 10% in this present work. The saturated liquid density shows the best accuracy in the prediction, with an AARD of 5.85%, where the absolute relative error of the saturated liquid density for more than half of the organic working fluids is within 5%. Besides this, it is clearly seen in Fig. 2 that the acentric factor has a large relative error. This is due to the fact that the expression for the group contribution to the acentric factor is determined by a combination of the boiling temperature and the critical properties of the organic working fluid. The value of the AARD of the acentric factor is 11.09%. For improvement in the accuracy of the prediction of the acentric factor, it is necessary to ensure an accurate estimation of the boiling temperature and critical properties.

Table. 2 The basic physical properties

ASRHAE	Tb(k)	Tc(k)	Pc(bar)	ω	ρ(kg/m³)
R123	300.20	456.83	36.6618	0.2819	1438
R125	227.00	339.17	36.1770	0.3052	1125
R134a	246.60	374.21	40.5930	0.3268	1167
R143a	226.00	345.86	37.6100	0.2615	885
R152a	248.50	386.41	45.1680	0.2752	873
R218	234.00	345.02	26.4000	0.3172	1260
R227ea	255.00	374.90	29.2500	0.3570	1344
R236ea	279.00	412.44	34.2000	0.3690	1393
R236fa	272.10	398.07	32.0000	0.3770	1324
R245ca	298.10	447.57	39.4070	0.3550	1361
R245fa	288.50	427.16	36.5100	0.3776	1310
R290	231.10	369.89	42.5120	0.1521	476
R600	273.00	425.13	37.9600	0.2010	561
R600a	262.00	407.81	36.2900	0.1840	537
R601	309.20	469.70	33.7000	0.2510	610
R601a	301.10	460.35	33.7800	0.2274	604
n-C6H14	341.90	507.82	30.3400	0.2990	645
C5F12	302.60	420.56	20.4500	0.4230	1578
R1233zd	291.47	438.75	35.7090	0.3050	1238
R1234yf	243.70	367.85	33.8220	0.2760	1054
R1234ze	254.18	382.51	36.3490	0.3130	1129

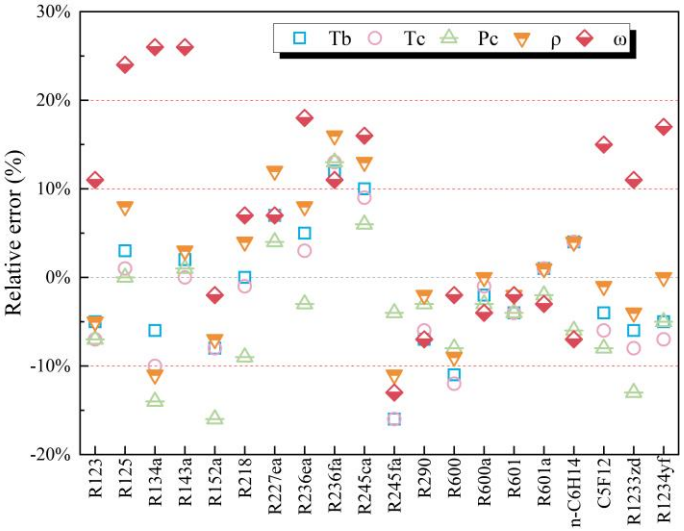

Fig.2 Relative error of the basic physical properties

3.2 Analysis of the thermodynamic performance

To ensure that the complete Rankine-based Carnot battery cycle is in the subcritical range, the critical temperature of the organic working fluid selected to evaluate the thermodynamic system performance should be greater than 378.15 K according to boundary conditions. Therefore, the whole system performance of the Rankine-based Carnot battery applying the 14 different working fluids (in Table . 3) including power-to-power efficiency, coefficient of performance, and power generation efficiency in this section.

Table. 3 The whole system performance

ASRHAE	COP	η_{orc}	P2P
R123	6.73	6.47%	41.38%
R152a	5.72	6.29%	34.19%
R236ea	5.97	6.18%	35.07%
R236fa	5.64	6.12%	32.74%
R245ca	6.53	6.37%	39.50%
R245fa	6.34	6.34%	38.19%
R600	6.27	6.32%	37.68%
R600a	5.90	6.22%	34.88%
R601	6.63	6.39%	40.25%
R601a	6.52	6.35%	39.29%
n-C6H14	6.76	6.41%	41.14%
C5F12	5.17	5.65%	27.73%
R1233zd	6.56	6.41%	39.92%
R1234ze	5.21	6.11%	30.20%

Fig. 3 presents the relative error distribution of the whole performance of the Rankine-based Carnot battery. It can be observed that the absolute relative error is less than 10% for most considered working fluids. The AARDs for power-to-power efficiency, coefficient of performance, and power generation efficiency are 8.5%, 5.9%, and 2.6%, respectively.

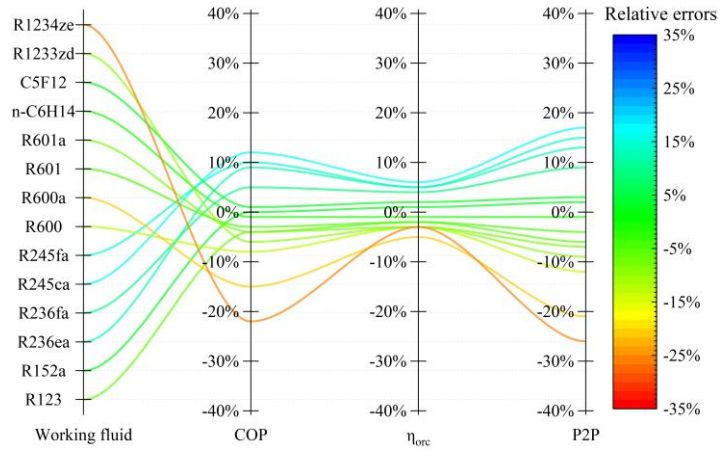

Fig.3 Relative error of the whole system performance

4. CONCLUSIONS

In this study, a model was developed based on the group contribution method that is used to prefer the working fluid of the Rankine-based Carnot battery, and this cross-scale model enables the study of the molecular structure, physical parameters, and system performance. The accuracy of the basic physical properties of 21 organic working fluids obtained from the cross-scale model presented in this paper is investigated. Furthermore, the predictive accuracy of the performance of the Rankine-based Carnot battery under different working fluids is further evaluated for specific operating conditions. The absolute average relative deviations of the basic physical properties of the 21 organic working fluids are 5.91%, 6.25%, 6.47%, 11.09%, and 5.85% in that order, respectively. The absolute value of the mean relative distribution error of the three thermodynamic performance criteria important for evaluating the performance of the system is 8.5%, 5.9%, and 2.6%, sequentially. Based on this, the model is considered to be accurate and can be used to subsequently guide the screening of the working fluid of the Rankine-based Carnot battery.

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