

A simultaneous approach to optimize the component and composition of zeotropic mixture for power generation systems



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ABSTRACT

The variable temperature characteristics of isobaric phase transition process for zeotropic mixture can effectively reduce the heat transfer irreversibility between working fluids and heat sources or heat sinks for thermodynamic cycle systems. One of the key problems in the application of zeotropic mixtures for power generation systems is how to determine their optimal components and compositions. The traditional method is mainly based on the exhaustive method, which means that every considered component and their compositions in the mixture are optimized one by one and mainly caused by the independence and discontinuity of components. This process will consume a large amount of computing resources, which limits the optimization of zeotropic mixtures. In order to describe the discrete components and optimize them, the selective coefficient representing every component alternative is introduced and this paper recommends a simultaneous approach to achieve the optimal components and compositions of zeotropic mixture at the same time. Two case studies with different heat sources and sinks as well as system layouts are illustrated to show the proposed approach. Besides, it also proves the systems with zeotropic mixture have better performance than that of systems with pure fluid.

1. Introduction

The use of low-temperature heat sources to generate electricity is one of means to alleviate the shortage of energy [1]. The main power generation technology for low-temperature heat includes organic Rankine cycle (ORC)[2–4], Kalina cycle [5] and flash cycle [6] and so on. The largest bottleneck of low-temperature power generation system is inherent inefficient. The irreversible loss of heat transfer process is an important factor restricting the efficiency of low-temperature power generation system.

The use of mixed working fluid is to utilize the variable temperature characteristics of isobaric phase transition process for zeotropic mixture, which can effectively reduce the heat transfer irreversibility between working fluid and heat sources or heat sinks for thermodynamic cycle systems [7–9]. It's considered that temperature matching in the condensation process had greater influence than that of the evaporation process when using zeotropic mixture [10–12]. Heberle et al. [10] found that the optimal composition of zeotropic mixture is related to the temperature rise of the cooling water. Similarly, Liu et al. [11] also pointed out the effect of the relationship between temperature glide of condensation process and temperature rise of cooling water on the optimal composition of zeotropic mixture. With three different restrictive conditions for the cooling conditions, including the bubble

temperature in the condenser, the temperature rise of cooling water and the flow rate of cooling water, Lu et al. [13] studied the effect of restrictive conditions on the evaluation of ORC systems with zeotropic mixture. They concluded that fixed cooling water flow rate is more suitable to select the zeotropic working fluids. Because the temperature change of heat source side is usually larger than that of the heat sink side, the transcritical Rankine cycles with mixed working fluid have also attracted a lot of attentions [14–17]. In addition, by mixing of different pure fluids, the weaknesses of different pure fluids could be reduced. For example, for hydrocarbons or siloxane flammable fluid, they can be added to the flame retardant [18–21], which makes up the safety properties of the mixture.

One of the key problems for mixed working fluids is to determine their optimal components and compositions. The early research mainly aimed at specific working fluids [22–24]. After a predefined group of components in a small range, for binary mixed working fluids, most of the research is to change composition between 0 and 1. By the change trend of the objective function in the whole concentration range, it could determine the optimal composition of mixtures [13,25–29]. There are also a few scholars using computer-aided molecular design (CAMD) and group contribution method to design the components and compositions of zeotropic mixtures [30,31].

There are some researches on the optimization of the components

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and compositions of zeotropic mixtures. For binary mixture, with R245fa as the flame retardant forming four mixed working fluids, Xi et al. [32] used Electricity production cost (EPC) as the objective function and optimized the composition of zeotropic mixtures by genetic algorithms. In order to utilize the geothermal energy of 100–150 °C, the transcritical Rankine cycle using CO₂ mixed with other fluids was studied by Wu et al. [33]. They used pattern search algorithm to optimize the composition of the zeotropic mixture and the objective function was the net power output. There are also some researchers focused on multicomponent mixtures. With high temperature and low temperature heat source as the research object respectively, Chys et al. [34] optimized the compositions of different binary and ternary mixtures. Their results showed that the performance of system with ternary mixture only increased a bit compared to that of system with binary mixture. Prasad et al. [35] used Aspen Plus software to optimize the compositions of multicomponent mixtures by the SQP method. The results showed that the mixed working fluids can guarantee a smaller size expander at the same exergy efficiency. With the net output power as the objective function, Satanphol et al. [36] also used the SQP optimization method to determine the optimal components, compositions and operating conditions for the basic organic Rankine cycle with mixtures. They found that a quaternary blend R-218/227ea/C318/245fa has the largest net work output. With the sum of the heat transfer temperature difference as the objective function, Lee and Mitsos [37] used a hybrid optimization approach to optimize the composition of ternary mixture. Recently, Santos-Rodriguez et al. [38] proposed a stochastic optimization approach to design the composition of mixture, including binary and ternary mixture, considering the variation of heat source temperature and efficiency of expander.

Based on the above literature review, most of the literatures are in the case of known components, and their compositions are optimized. There is also a small amount of literature to optimize different component and their compositions one by one, and then the optimal value is obtained by comparing the optimal performance of all the mixture considered. So the contribution of this paper is as follows: Through the introduction of selective coefficient, a simultaneous approach to achieve the optimal components and compositions of zeotropic mixture at the same time is recommended. Firstly the methodology is introduced, including the basic idea of the proposed approach, problem definition and optimization details. After that two cases with different heat sources and sinks as well as system layouts are illustrated to show the proposed approach.

2. Methodology

2.1. Basic idea of the simultaneous approach

As the review of the introduction part, the traditional method of determining the components and compositions of mixtures is firstly to predefine some fluids, and then, according to the number of components, these fluids are chosen and combined as the component of mixed working fluids one by one. At last, the compositions of the formed mixtures and the corresponding system parameters are optimized at the specified system structure respectively. Fig. 1 shows the direct relationship between the number of calculations and the total number of preselected components at different number of component for mixed working fluids. It can be seen that with the increase of the total number of preselected components and number of component for mixed working fluids, the number of calculations will significantly increase, which means that the determination of the optimal component and composition for mixtures will be a difficult task and challenge.

It is difficult to optimize the components of a mixture, because the components of the mixed working fluids are independent of each other and discrete, and meanwhile it is difficult to describe them with mathematical variables. In order to reduce the intensity of calculation for components and compositions of zeotropic mixtures and achieve the

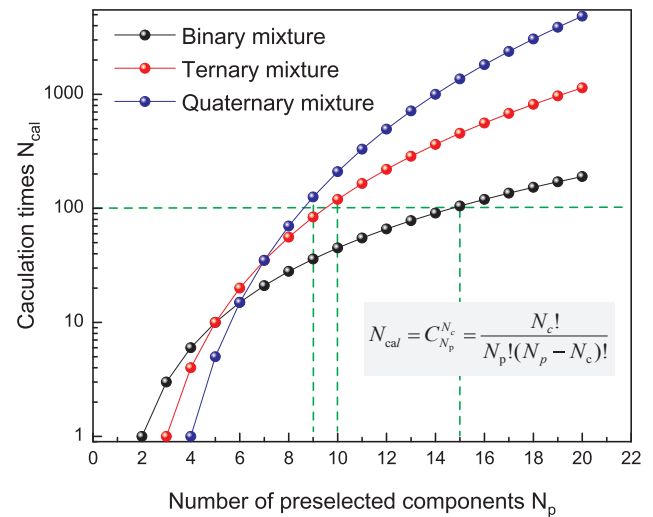


Fig. 1. The change tendency of the number of calculations with the total number of preselected components at different number of component for mixed working fluids.

Component Selective Composition coefficient

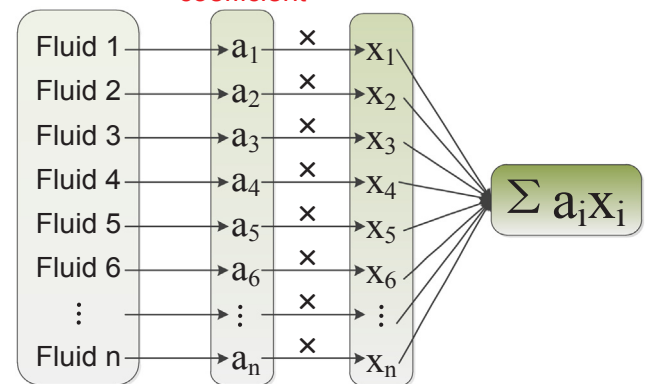


Fig. 2. Basic idea for simultaneous approach to optimize component and composition of zeotropic mixture.

simultaneous optimization of components and compositions for zeotropic mixtures, this paper introduces a selective coefficient a_i , as shown in Fig. 2. Because the components of mixture are discrete, only discrete variables can be used to describe them. Each component of mixture is expressed by a selective coefficient. The selective coefficient a_i is a binary variable, and it has two values 0 or 1. When the value of selective coefficient a_i is 1, the component expressed by this selective coefficient is selected. While the value of selective coefficient a_i is 0, it means this component is not selected. The sum of the selective coefficient a_i is used to control the number of component for mixture. For example, binary mixture can be optimized by $\sum a_i = 2$. While the composition x_i of each component is the continuous variable and its value is between 0 and 1. There are no constraint conditions for composition x_i , but the total sum of compositions for all the selected components should be 1, i.e., $\sum a_i x_i = 1$.

2.2. Problem definition

In order to realize the simultaneous approach to design the components and compositions for mixtures in Section 2.1, the following mathematical programming problem of Mixed-Integer Nonlinear Programming (MINLP) is formed:

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