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Optimization-Based Design and Selection of Working Fluids for Heat Transfer: Case Study in Heat Pipes

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Ⓢ *Supporting Information*

ABSTRACT: In this paper, an in silico methodology for optimizing/designing working fluids for heat transfer is presented. The method is tested for heat pipe fluids using a validated model of an evacuated tube solar water heater as a case study. Two model modes are assessed: one simplistic temperature-independent mode and one more complex temperature-dependent mode. The method demonstrates successful optimization of working fluid properties rapidly leading to optimal design of real working fluid mixtures, thus avoiding laborious and time-consuming trial-and-error experimentation. Simulations of solar water heaters with optimized working fluids lead to overall performance improvements in the order of 40%.

1. INTRODUCTION

Working fluids are industrially ubiquitous and are at the heart of many heat transfer processes. They have significant impact on process design, operation, and economics. Identifying optimal working fluids/media or predicting the features of the optimal working fluids/media is therefore a big concern in the strive for ever more efficient processes.

Researchers have reported the use of Computer Aided Molecular Design (CAMD) or in silico approaches for the computation of optimal material properties or for structural predictions of solid as well as liquid phase materials, such as for solvent design.[1−6] However, less attention in the literature has been given to computational-based or optimization-based determination of heat transfer fluids, and more specifically, working fluids in heat pipes. Several experimental attempts have been made to optimize the working fluid for heat pipes or devices that use heat pipes;[7−26] however, these attempts are mostly based on trial-and-error and do not design the working fluid prior to testing. Although some insights have emerged through the systematic improvement of working fluid properties,[8,27,28] they can be treated as working fluid modification rather than working fluid design or optimization.

In a recent work, we presented a detailed modeling treatment of the heat pipe and observations about the behavior of the heat pipe while changes in the working fluid properties and type are applied.[32] That work also presented a dimensionless analysis that reduces the dimension of the heat pipe system. In a sequel,[31] we applied the heat pipe model in the specific application of solar water heaters, validated the dynamic model, and presented the effect of manipulating the working fluid through the use of a hypothetical fluid. We also presented the economics and operation of the solar water heater in detail during a typical year in Sydney, Australia. In this current paper, an in silico optimization-based methodology is presented that can be used to predict the components and compositions of an optimal working fluid in heat pipes. Such a methodology has generic importance not only because it transcends across a myriad of applications like heat pipes, but also because it directs the material designer toward a target set of fluid/material properties, regardless of whether the manufacturing method of that fluid/material is already developed or not. In other words, it is possible to predetermine optimal properties of a working fluid within a hypothetical property range that would achieve given process performance criteria. This methodology therefore builds reverse calculation between fluid properties and process design. Equation-based models consisting of integro-differential-algebraic equation (IDAE) systems are at the core of this methodology. The complexity inherent in these equation systems leads to convergence issues when attempting to optimize the working fluid/media direct by use of the said models. This can be avoided by the methodology that is described here, whereby the optimization is divided into two steps; the first determines the optimal fluid/material property set, whereas a real mixture is subsequently matched to that optimal set in the second step.

To make it clearer, the proposed methodology is compared in Figure 1 with the traditional procedure. Steps 1 and 2 in the traditional procedure (Figure 1a) are highly heuristic, and step 3 is costly and time-consuming; especially if this is to be experimentally tested for every possible working fluid. Moreover, the performance of the selected working fluids is highly affected by the selected fluid mixture components as well as their compositions. For example, assume the designer chooses to test additive A and water as components of the working fluid. This combination might work better than pure water at very low concentrations (less than 3%) but may not work very well at higher concentrations (higher than 10%). So if suboptimal compositions are selected in step 2, then the results of the tests in step 3 will also be consequently suboptimal. The proposed procedure in this study (Figure 1b) drastically reduces the number of experimental tests required. This is achieved through screening a large number of candidate working fluids and solely selecting the most promising mixtures for further study or

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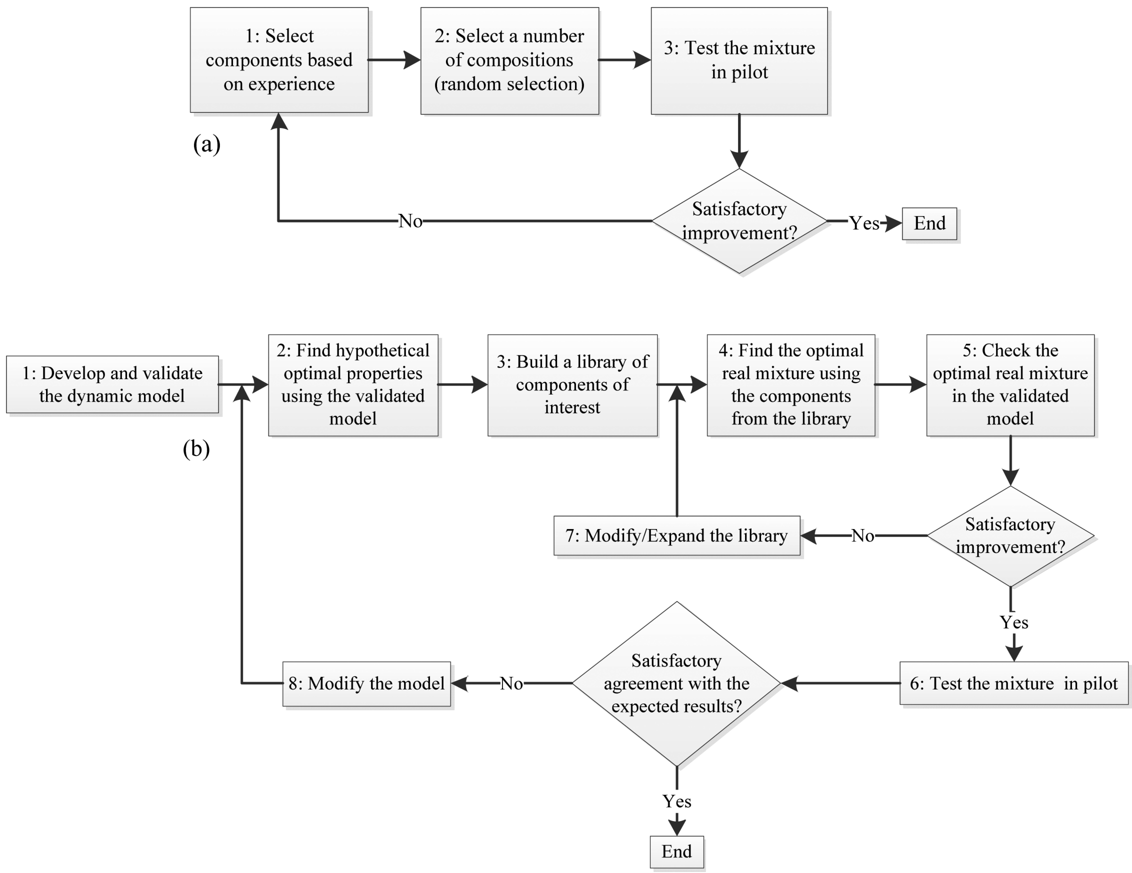

Figure 1. (a) Traditional working fluid optimization procedure versus (b) working fluid design and selection procedure proposed in this study.

validation. It also proposes a computed and therefore meaningful concentration for each component set to guide the experimental tests. Experimental trial-and-error is therefore minimized and optimal results are more likely to be realized. In addition, the selection of suitable components to build the component library in step 3 can be well guided by the fact that the optimal properties are already known from step 2. Furthermore, experience can be gained more quickly and be applied more easily during the design steps. Therefore, if the designer finds out specific types of components work better in the simulation steps (steps 4 and 5) or from other sources of information, then the component library can be modified or expanded accordingly (step 7) to include the new possibilities.

To study the performance of the proposed procedure, we used an experimentally validated dynamic mathematical model of an evacuated tube solar water heater (SWH). The model is simulated for "specific input parameters" including location-specific weather data and for a specific SWH with built-in grooved heat pipes. An optimization procedure is then formulated using genetic algorithm (GA) and pattern search algorithm (PS) utilizing the Global Optimization Toolbox of MATLAB (Mathworks, USA). This optimization formulation is executed subject to the model and to the specific input parameters. The result of the optimization is expected to be one or more optimal working fluid mixtures that would perform best within the range of specific input parameters. As such, the optimally computed working fluid mixture is optimal for the given conditions and is such optimal within the given geographical location and SWH system parameters. Once the optimal fluid mixture and its composition are computed, we proceed to test its performance via simulation of the validated dynamic model of the SWH system. Improvements in performance are measured through the total thermal resistance and the critical heat flux of the heat pipes. Such technical performance criteria are followed by an economic performance analysis of the entire system. The above-mentioned computational analysis, i.e., the optimization-based design and selection of working fluids, is performed in two modes namely temperature-dependent (TD) mode and temperature-independent (TiD) mode. Flowcharts detailing the steps in these two modes are shown in panels a and b in Figure 2, respectively.

2. METHODOLOGY

2.1. Scenario Description. To run the optimization-based design of the working fluid, we defined a scenario (scenario A) based on the requirements of a 5-member family. The schematic diagram of the simulated SWH system is shown in Figure 3. In this scenario, a total number of 20 heat pipe evacuated tubes are considered in the SWH. The hot water drain mass flow rate varies on an hourly basis based on hot water consumption pattern of a typical household as shown in Figure 4. Typical weather data for the first day of January in Sydney, Australia, is used (Figure 5). The technical details of scenario A are described in Section 2.2.

2.2. Technical Details of Apparatus. To undertake a realistic study, we assumed a hot water tank with storage capacity of 470 litters. This storage capacity is sufficient to meet the hot water demand of a 5-member family for 24 h. A dynamic model previously developed for this purpose is used.

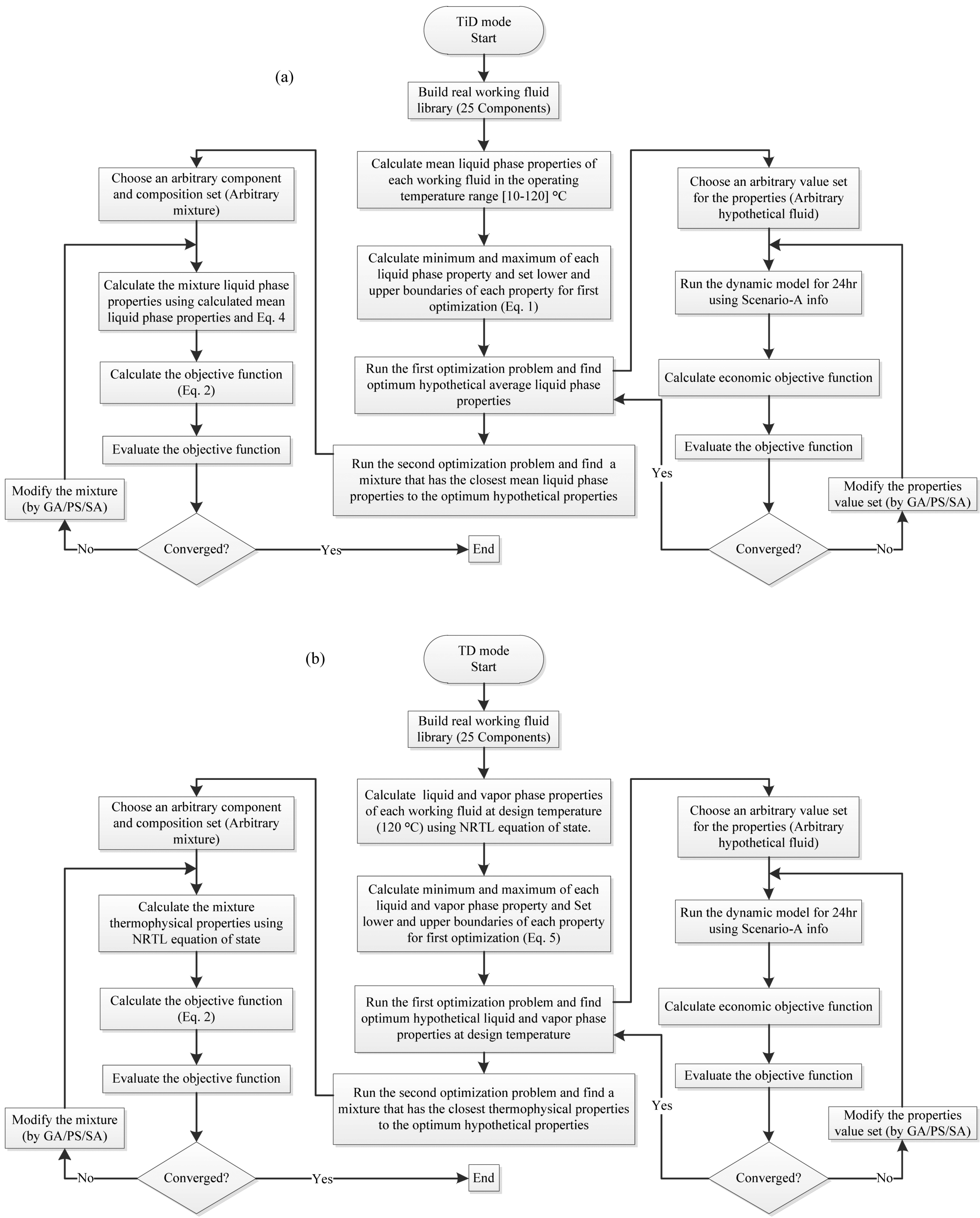

Figure 2. Flowchart of the optimization problem in (a) temperature-dependent (TD) mode and (b) temperature-independent (TiD) mode.

The model is validated against experimental data.[32,31] As shown in Figure 3, like most real hot water systems, it is assumed that the water circulates in a closed loop in contact with the evacuated tubes and at a constant rate of 0.033 kg/s. Assuming that the hot water is being consumed during 24 h of the typical day according to the pattern shown in Figure 4, fresh water flows inside the hot water tank at the same rate, substituting the consumed hot water and keeping the total volume/mass of water in the tank constant during the day. As a result, the cold fresh water mixes with the hot water in the tank. The dimensional information of the heat pipes and the evacuated tube SWH are presented in Tables 1S and 2S in the Supporting Information. The total length of the connecting pipes is assumed to be 4 m (connecting pipes are the piping used to connect different components of the solar water heater). The tank and all connecting pipes including manifold are insulated by 10 cm thick glass wool.

2.3. Optimization Algorithm. The optimization problem is run for two modes. In the first mode, temperature-independent mode (TiD mode), the purpose of the optimization is to find a real fluid which has the closest mean liquid phase properties to that of the global hypothetical optimum fluid. In the second mode, temperature-dependent mode (TD mode), a design temperature based on the

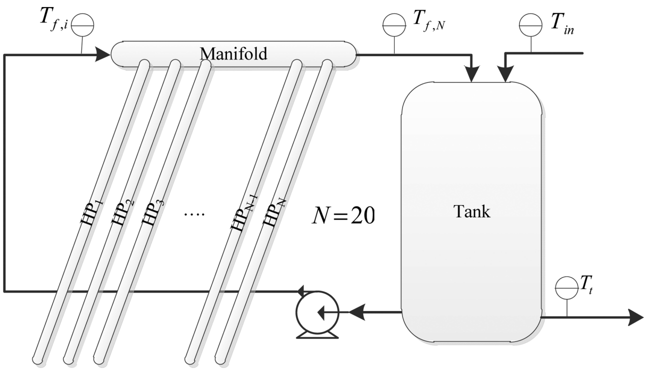

Figure 3. Schematic diagram of modeled evacuated tube solar water heater with N heat pipes.

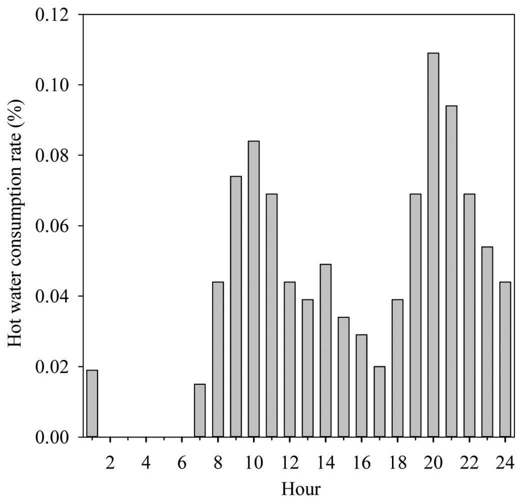

Figure 4. Hot water consumption pattern in a typical household during 24 h of a typical day.[29]

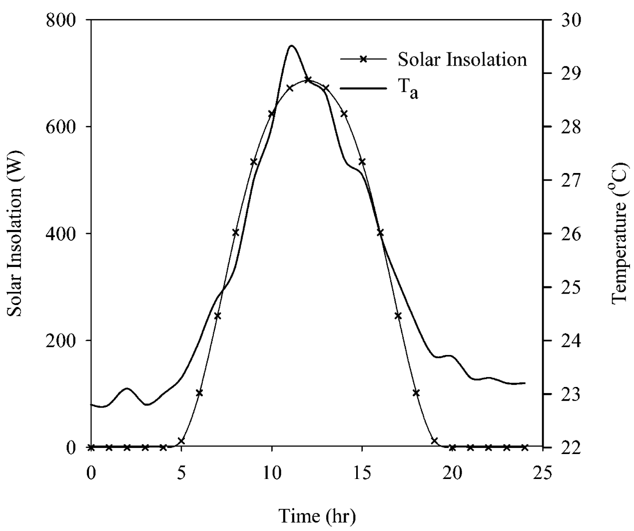

Figure 5. Typical Sydney weather data on the first day of January.[30]

temperature profiles obtained from the dynamic simulation of the evacuated tube SWH is defined. The working fluid properties including the vapor phase properties are optimized at that design temperature, which is 120 °C in this study. Recall that the final goal of the optimization is to identify a mixture of predefined real fluids which has the closest properties to that of the global hypothetical optimum fluid. Therefore, two main differences exist between the two studied modes: dependence/independence of working fluid properties on/from temperature, and including/excluding vapor phase properties in the optimization problem.

As shown in Figure 2, the optimization problem in each mode is divided in two further steps. The first step is to find the optimal values for fluid properties, and the second step is to find a mixture of real fluids that best matches the optimized properties. Pattern Search and Genetic Algorithms are applied to the first step in order to find the best algorithm and to make sure the final optimization solution is a global one. However, for the second step, only GA is applied because of restrictions that are inherent to the PS method.

The use of GA optimization approach is because it can handle the complex nonlinearities in the mathematical model. Such a model, which is also a dynamic one, is like an egg carton in terms of objective function behavior, where it exhibits many local optima. It is well-known that classical optimization techniques do not perform well in such a situation. Second, the model is based on numerical solution of a DAE system, which makes it almost impossible to calculate gradient matrices as required by classical optimization approaches. Third, the second optimization problem presented is of the mixed integer optimization type; changes in working fluid components represented by integers as part of the optimization manipulated variables drastically change the thermophysical properties and temperature functionality of the mixture. Situations like this should avoid the use of classical optimization methods. Finally, we tested a couple of classical optimization methods and found that if the algorithm manages to converge to a specific point (which does not happen very frequently), the final optimal solution would highly depend on the starting point. So, all in all, using global optimization methods like GA and checking the reproducibility of the results is an appropriate approach to deal with such a problem.

A more detail description of the optimization problems is provided below.

2.3.1. TiD Mode (Mean Liquid Phase Properties). For TiD mode, there are two separate optimization problems to deal with, one for each step (see Figure 2a).

- For the first optimization problem, three different global optimization algorithms, Simulated Annealing (SA), Genetic Algorithm (GA), and Pattern Search (PS), have been tested to find the best mean liquid phase properties of the working fluid. The performance of SA was not satisfactory for this problem therefore the results are not presented here. GA and PS provided good responses in finding the optimal values.
- For the second step, a lookup table consisting of 25 most common fluids in heat transfer has been used (for the list of fluids refer to the Supporting Information). GA is applied to the problem to find the best combination of the 25 working fluids targeting the prior stage results. For this step, average properties have been used and mixtures are assumed to be ideal

2.3.2. TD Mode (Vapor and Liquid Phase Properties at Design Temperature). The procedure that is used in this mode (see Figure 2b) is similar to the TiD mode. However some important differences exist as below:

- For the first step, vapor phase properties are also considered in the TD mode. In addition, optimization is run at 120 °C as design temperature. Therefore, temperature dependence of the working fluid properties is considered by optimizing the properties at a specific temperature which is the maximum operational temperature of the heat pipes at the specific input parameters. This maximum temperature has been chosen based on previous simulation runs[32] using different working fluids and the maximum desirable operating temperature for the heat pipes for this specific heating application.

– For the second step, a lookup table consisting of the same 25 most common fluids in heat transfer has been created. GA is applied to the problem to find the best combination of the 25 working fluids targeting the results of the prior stage. To keep the optimization as close as possible to the real phase transitions occurring inside the heat pipe, we integrated the optimization code to a HYSYS (Aspentech, USA) process model through COM Server, to calculate fluid properties through NRTL equation of state inside Aspen plus databank. Therefore, deviations from ideal fluids both in liquid and vapor phases (effect of reduced properties), variation in the thermophysical properties due to variation of the composition in liquid and vapor phase, and change in the thermophysical properties due to working fluid operating temperature are all taken into account.

2.4. Objective Function and Restriction. *2.4.1. TiD Mode.* Generally, by optimizing the working fluid, we expect to observe reductions in total thermal resistance of the built-in heat pipes and as a result the efficiency of the SWH will increase. On the other hand, we expect to observe an increase in the CHF of the heat pipes, which is closely related to the maximum heating capacity of the SWH. Therefore, by using an improved (optimized) working fluid in a typical SWH, it would be possible to harvest considerably higher amounts of solar energy.[32]

However, as mentioned in our previous work,[31] all actions that can be taken to improve the CHF work against improvement of the thermal resistance. Nevertheless, thermal conductivity is an exception in this case since based on the applied theoretical model, described in detail in,[31] the CHF solely depends on hydrodynamic behavior of the working fluid. Anyhow, to combine and consider both technical criteria (i.e., thermal resistance and CHF) for optimization, defining an objective function in the form of systems economics seems suitable. Therefore, for the first optimization problem the objective function (which is referred to as the first objective function throughout this paper) is the operating cost of the SWH. This cost is the price of the electricity consumed to meet the demand of the household plus a penalty that will be imposed if the SWH fails to operate because of critical heat flux violation. The aim is to minimize the objective by manipulating the mean thermophysical properties of the liquid phase, namely σ, h_{fg}, k, μ_l, and ρ_l. The limits for thermophysical properties of the liquid phase are defined based on the maximum and minimum of the mean values of the properties for the considered working fluids in the temperature range of (10–120) °C as shown in eq 1.

For the second optimization problem, which is to find the best components and compositions of the working fluid mixture, the objective function is the sum of squares of the properties ratio over target values which represents the proximity of the working fluid properties to the target/optimized values (eq 2). For this problem, the decision variables are the discrete components themselves and the nondiscrete mole fractions of each component in the working fluid mixture. The restrictions are shown in eq 3. The properties of the liquid phase of the mixture are calculated by eq 4 assuming the mixture as an ideal liquid.

constraints:

$$\begin{aligned}
&0.0015 < \sigma < 0.0728 && (\mathrm{N m^{-1}})\\
&0.27 \times 10^6 < h_{fg} < 2.444 \times 10^6 && (\mathrm{J\,kg^{-1}})\\
&0.12 < k < 0.683 && (\mathrm{W\,m^{-1}C^{-1}})\\
&0.07 \times 10^{-3} < \mu_l < 1.7 \times 10^{-3} && (\mathrm{Pa\ s})\\
&374 < \rho_l < 998 && (\mathrm{kg\,m^{-3}})
\end{aligned} \tag{1}$$

$$\mathrm{obj}_{\mathrm{property}} = \sum \left(\frac{\mathrm{property}_{\mathrm{opt}} - \mathrm{property}_{\mathrm{mix}}}{\mathrm{property}_{\mathrm{opt}}} \right)^2 \tag{2}$$

subject to:

$$0 \le x_i \le 1 \tag{3}$$

$$\mathrm{property}_{\mathrm{mix}} = \sum_{i=1}^{N=25} x_i \times \mathrm{property}_i \tag{4}$$

2.4.2. TD Mode. In terms of the applied objective functions, the only difference that exists in the TD mode in comparison to the TiD mode is related to upper and lower limits of each thermophysical property. The limits for thermophysical properties of liquid phase are defined based on the maximum and minimum of the properties for the working fluids included in the library at 120 °C. The limits are shown in eq 5. The objective function for the first and second optimization step in this mode are the same as the TiD mode.

constraints:

$$\begin{aligned}
&0.00368 < \sigma < 0.0243 && (\mathrm{N\,m^{-1}})\\
&127 \times 10^3 < h_{fg} < 2200 \times 10^3 && (\mathrm{J\,kg^{-1}})\\
&0.0607 < k < 0.684 && (\mathrm{W\,m^{-1}C^{-1}})\\
&0.0486 \times 10^{-3} < \mu_l < 0.669 \times 10^{-3} && (\mathrm{Pa\ s})\\
&7.86 \times 10^{-6} < \mu_v < 22.2 \times 10^{-6} && (\mathrm{Pa\ s})\\
&374 < \rho_l < 1290 && (\mathrm{kg\,m^{-3}})\\
&0.445 < \rho_v < 206 && (\mathrm{kg\,m^{-3}})
\end{aligned} \tag{5}$$

3. RESULTS AND DISCUSSION

3.1. TiD Mode. *3.1.1. Thermophysical Properties.* The trends of the objective function through optimization using each one of the mentioned methods (GA and PS) are shown in Figures 6 and 7. Negative values for the objective function means the heat demand of the household has been met and the CHF of the heat pipes are high enough and as a result the SWH works smoothly. In addition, it is desirable to have more negative objective function values, which means the SWH is more efficient.

To make sure the optimal values are not local optima each method is run several times. For PS several starting points have

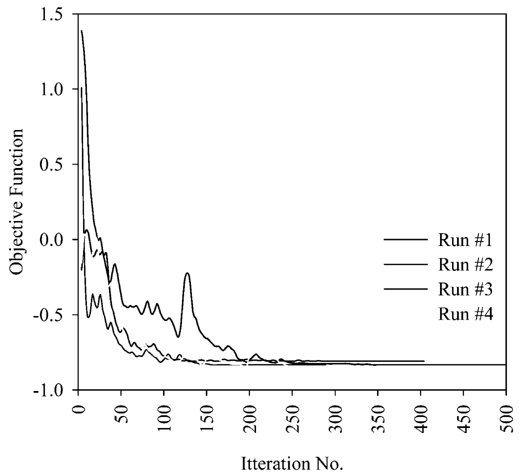

Figure 6. Trend of the objective function using PS as the optimization method for TiD mode (Note: the values are smoothened using spline method for better presentation quality).

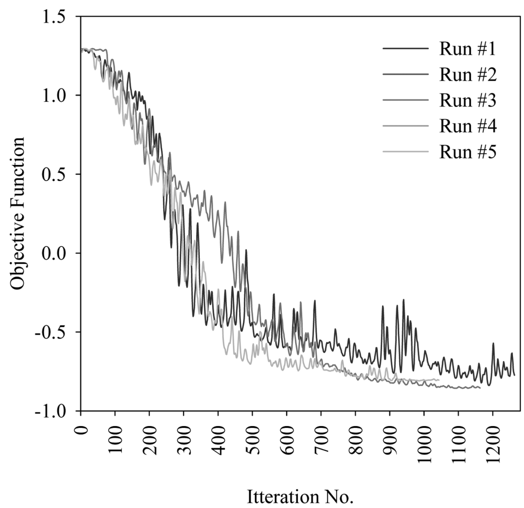

Figure 7. Trend of objective function using GA as the optimization method for TiD mode (Note: the values are smoothened using spline method for better presentation quality).

been selected as shown in Table 3S in the Supporting Information. As shown in Figure 6, the result of the optimization problem is only slightly affected by varying the starting point. In addition, several runs of GA with different sets of random first generations also show very slight difference in the optimal value of objective function (Figure 7). In other words, the probability of reaching to the global optima is very high in this step. Therefore, it can be concluded that for the TiD mode, PS and GA optimization methods seem to be suitable. However, the optimization problem is very sensitive to the form of objective function. It is worth noting that the results of GA are marginally better than that of PS, however, they require more iterations and consequently longer CPU-time to find the optimal values (1500 iterations for GA vs 500 iterations for PS). The final values of thermophysical properties for each run are shown in Table 1.

Analyzing the final optimized properties for each run provides us with some insight into liquid phase optimization. For latent heat, thermal conductivity, surface tension, and liquid phase density, the optimizer (GA or PS) tends to choose values that are close to the upper limits. For liquid phase viscosity, the optimizer chooses values that are close to the lower limit. This is consistent with the concept of figure of merit (eq 6). It means the optimizer algorithm tries to increase CHF as much as possible. The main reason for this behavior is that there is a huge cost penalty for heat pipe failure, which is an order of magnitude higher than the penalty for increased thermal resistance of heat pipes (refer to Section 2.4.1). However, when comparing very similar working fluids, the mentioned figure of merit may not be very accurate.[32]

$$\text{figure of merit} = \frac{\rho_1 \sigma h_{fg}}{\mu_1} \quad (6)$$

3.1.2. Composition. The result of the previous section is a hypothetical working fluid with optimized properties which are still far from a real world fluid. However, the optimized properties can guide the discovery of a real optimized working fluid. To do so, among the properties that are mentioned in Table 1, the result of the second run of GA (GA #2) is used as target values because of its best objective function and proven better performance on annual basis as described in ref 32. To find out the best combination/mixture of working fluids, we executed the second step of optimization problem as described in Section 2.4.1. The objective function is presented in eq 2, and the results are shown in Table 2.

Table 2. Components and Composition of the Optimized Real Fluids for TiD Mode (compositions shown in brackets)

no. of components	component #1	component #2	objective function[a]
2	22 (0.13)	21 (0.87)	1.6355
	22 (0.13)	21 (0.87)	1.6355
	22 (0.13)	21 (0.87)	1.6355
	22 (0.13)	21 (0.87)	1.6355
	21 (0.77)	22 (0.23)	1.6355

[a]The value of objective function for pure water is 13.8297.

Table 1. Optimal Thermophysical Properties Resulted from Applying PS and GA for TiD Mode

	run	h_{fg}	ρ_l	k	μ_l	σ	objective function
PS	#1	2.44×10^{06}	864	0.459	1.25×10^{-04}	0.0728	−0.833
	#2	2.43×10^{06}	898	0.550	1.00×10^{-04}	0.0719	−0.810
	#3	2.44×10^{06}	681	0.655	7.00×10^{-05}	0.0726	−0.833
	#4	2.45×10^{06}	884	0.649	7.00×10^{-05}	0.0726	−0.856
GA	#1	2.31×10^{06}	957	0.634	1.25×10^{-04}	0.0713	−0.671
	#2	2.45×10^{06}	971	0.644	9.86×10^{-05}	0.0727	−0.856
	#3	2.45×10^{06}	971	0.644	9.86×10^{-05}	0.0727	−0.856
	#4	2.43×10^{06}	953	0.474	1.48×10^{-04}	0.0724	−0.810

Theoretically, the best objective function value is zero, which represents a working fluid that 100% matches the optimized thermophysical properties. The calculated objective function for pure water (which is 13.8297) suggests that adding some additives to water can make it much closer to the optimal working fluid in terms of liquid phase properties. The results propose that real components 22 and 21 are definitely the best components that suit the target values. However, there is little variation in the compositions, which suggests a requirement for executing a further detailed optimization using the dynamic model and these two components to find the best global compositions. It is worth reminding that for the second step of the optimization, the optimizer is restricted to choosing just two components. Other number of components is also attempted (3 and 4 components). However, the optimizer was found to choose the same combination of components repeatedly.

To validate the optimization results of this mode (TiD mode), we used the computed working fluid mixture in the dynamic model directly to compare its performance against the performance of water. The result of this comparison is discussed in Section 3.3.

3.2. TD Mode. *3.2.1. Thermophysical Properties.* The optimization was executed and the trends of the optimization using each one of the mentioned algorithms are shown in Figure 8. For PS several starting points have been selected as shown in Table 4S in the Supporting Information. Again, the result of the optimization problem is only slightly affected by varying the starting point. In addition, GA reached the same final point. Therefore, it can be suggested that for the TD mode, PS and GA optimization methods also seem to be suitable. However, as in the TiD mode, PS reaches the final values much faster than GA. The optimized values of thermophysical properties for each run are shown in Table 3.

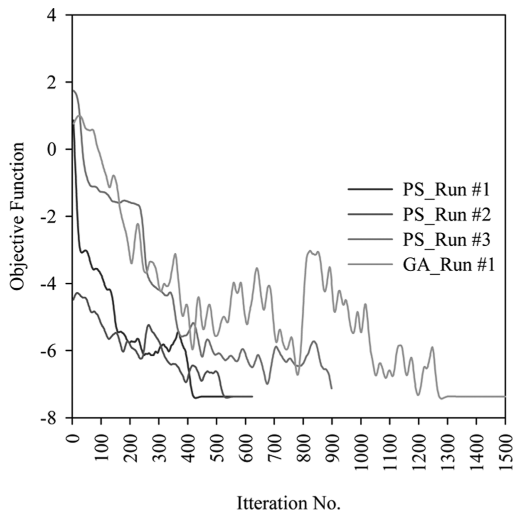

Figure 8. Trend of objective function using PS and GA as the optimization methods for TD mode (Note: the values are smoothened using spline method for better presentation quality).

As can be concluded from Table 3, for liquid phase properties, the optimization again leads to the properties which increase the figure of merit (eq 6). For the vapor phase, the optimizer tends to choose lower viscosity and higher density. Since all the performed optimizations converged to the same values, more runs were not conducted and reported here. For the next step of this mode the results of PS #1 are chosen as the target values.

3.2.2. Composition. The results of component and composition optimization (the second step) using GA are presented in Table 4.

Table 4. Components and Compositions of the Optimized Real Fluids for TD Mode (compositions shown in brackets)

no. of components	component #1	component #2	component #3	objective function[a]
2	22 (0.85)	5 (0.15)		2.5366
	22 (0.97)	5 (0.03)		2.5366
	6 (0.29)	22 (0.71)		2.0229
	22 (0.85)	5 (0.15)		2.5366
	22 (0.52)	6 (0.48)		2.0228
	6 (0.49)	22 (0.51)		2.0228
	22 (0.51)	6 (0.49)		2.1581
3	22 (0.51)	6 (0.40)	7 (0.08)	2.0402
	6 (0.46)	7 (0.03)	22 (0.51)	2.0299

[a]Objective function for pure water is 2.6127.

In this case also different number of components was chosen to carry out the optimization. As shown in Table 4, again two-component fluids are performing better than more complicated fluids. Although the optimizer chooses different set of components as the final solution there are two things to mention here: first, component 22 is always among the best set; second, there is always one lighter fluid (like component 5, 6, or 7) to modify the properties of component 22. In this case, considering the value of objective function for component 22, which is 2.6127, the final solutions are always better than component 22 itself but not as much as they were in TiD mode. The main reason is due to the specific vapor properties of component 22 at the design temperature. This shows the importance of considering the vapor phase properties in choosing the working fluid. This aspect is completely ignored by literature in working fluid optimization of heat pipes. The fluid mixture composed of components 22/6 always performs better than the 22/5 set for two-component fluids. Adding more components to the mixture does not improve the performance of the final fluid.

3.3. TD Mode vs TiD Mode. To find out to what extent the presented optimization method is effective to select the correct components and compositions, we integrated the dynamic model with the thermodynamic models existing in

Table 3. Optimal Thermophysical Properties Resulted from Applying PS and GA for TD Mode

	run	h_{fg}	ρ_l	k	μ_l	σ	ρ_v	μ_v	objective function
PS	#1	2.19×10^6	1286	0.6250	0.000544	0.0241	195.3	9.3×10^{-6}	−7.37227
	#2	2.2×10^6	1290	0.6332	0.000554	0.0243	182.1	10.9×10^{-6}	−7.37221
	#3	2.2×10^6	1290	0.6631	0.000049	0.0243	1.1	7.9×10^{-6}	−7.37234
GA	#1	1.22×10^6	1225	0.1818	0.000198	0.0184	32.3	10.7×10^{-6}	−7.3710

Aspen-HYSYS to calculate the thermophysical properties of the working fluid mixture for both liquid and vapor phases. This hybrid simulation is then run for the typical day using two best working fluid mixtures from TD mode (selected from Table 4) and one best working fluid mixture from TiD mode (selected from Table 2) and the behavior of the heat pipes are discussed below. The selected mixtures are shown in Table 5. To reduce the complexity of the discussion, only the simulation results of HP_{10} (the 10th heat pipe of the 20 built-in heat pipes) is presented (shown in Figure 9) and discussed here.

Table 5. Selected Mixtures for Comparison Study between TD Mode and TiD Mode

ID	mode	component #1	component #2
mix #1	TD	22 (0.97)	5 (0.03)
mix #2	TD	6 (0.29)	22 (0.71)
mix #3	TiD	22 (0.13)	21 (0.87)

In Figure 9, the gray dashed line shows the total thermal resistance and the CHF of the heat pipe filled with water. Water is chosen here to compare the results with due to the fact that it is one the best pure working fluids for heat pipes in the operating temperature range of interest.[32] Other lines show the total thermal resistance and the CHF of the same heat pipe filled with other computed working fluids relative to water. As can be seen for the TD mode, as far as this study is concerned, the final proposed mixtures work better than water both in terms of the thermal resistance and the critical heat flux. Especially the binary mixture of water and component 5 has very low thermal resistance just slightly higher than water (less than 5%) while bringing much higher heat transfer capacity (over 40% improvement). For TiD mode (mix #3), it is obvious that although the CHF is much higher than water and other mixtures in most times during the day, it also has much higher total thermal resistance in comparison to other mixtures and water (more than 2-fold), and has lower CHF in comparison to the other mixtures at the design temperatures (which is 120 °C and happens at the peak hour of solar insulation around 12 pm, see Figure 5), although it is higher than water. This shows that doing optimization in TiD mode in which the vapor phase properties are not included cannot provide us with the desirable result, which is simultaneous lower thermal resistance and higher critical heat flux.

However, it is worth mentioning that between the proposed mixtures by TD mode optimization (Table 4) there is an inconsistency between the achieved objective function values, which reflects the combined effect of the thermal resistance and the CHF of the heat pipe in economic terms, and the real performance of the mixtures in the dynamic model, which shows the effect of changing working fluid solely from a technical point of view. For example, for 22/5 mixture the optimized objective function value is 25% higher/worse than that of 22/6 mixture, whereas as shown in Figure 10, the economic objective function value of 22/5 mixture is 20% higher/better than that of 22/6 mixture. This fact suggests that the form of the objective function also needs to be improved to deliver the most desirable results. Anyhow, the nature of the optimization is such that a small variation in optimizing variables may lead to huge change in the objective function value. For example, if the optimizer replaces component 5 with 6, although there is a small change in the value in comparison to the given range (which is 1−25 while each number represents a different working fluid), the resulted change in the CHF and the total thermal resistance may be huge, resulting in huge difference in the calculated objective function.

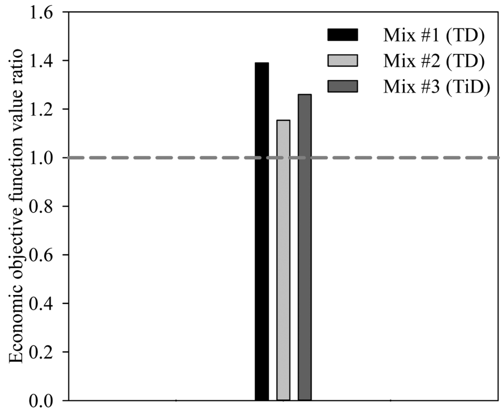

Figure 10. Economic objective value of optimized mixtures relative to water.

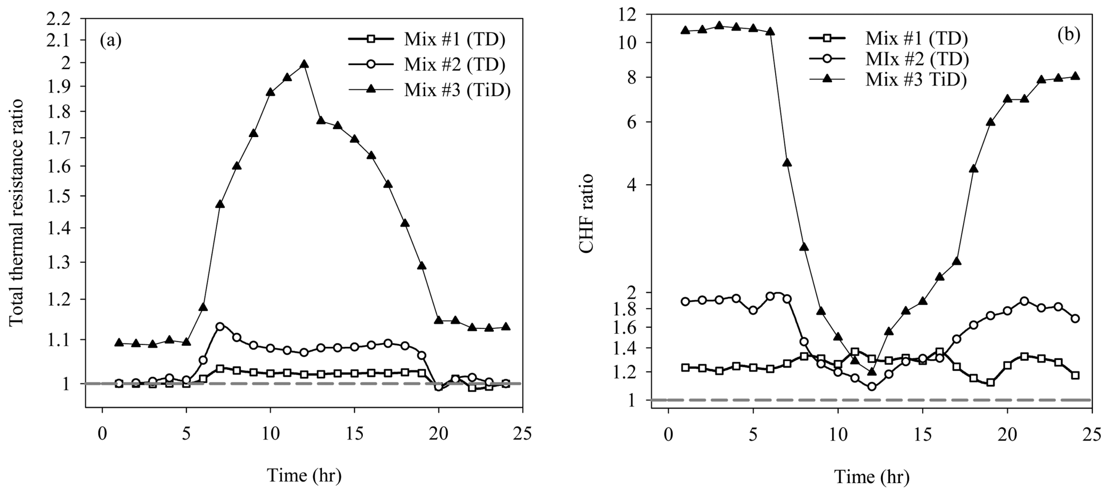

Figure 9. Total thermal resistance and critical heat flux ratio of optimized working fluids relative to water (HP_{10}).

Arranging the components in the working fluid library by molecule size or functional groups in order to reduce sudden changes in the components nature by changing the component number/ID might reduce the risk of improper selection or divergence. However, the effectiveness of the results suggests that the current form of the objective function is close to the optimal form, because it selects correct components and suggests a composition to start with for further experimental analysis and implementation.

4. CONCLUSION

In this study, the thermophysical properties of working fluids in an evacuated tube SWH are optimized in silico using two different modes focusing on temperature dependence and the effect of vapor phase properties. A common fluid component (component 22) emerged in all the final optimized real mixtures as one of the main components. This shows that component 22 is an ideal base fluid for the SWH system within specific input parameters. However, adding just a small amount of other fluids was shown to lead to much better performance. Using the real mixtures proposed by TD and TiD modes in the dynamic model shows the overall economics of the system can be improved by around 40% by adding 3% component 5 to the base fluid. Therefore, the proposed in silico computational method was shown to be very effective in screening a large number of potential heat transfer fluids and selecting a "best" component set for further optimization. This optimization-based method can rapidly provide initial compositions for the "best" set of components directing and expediting further experimental testing. The method was successfully applied to heat pipes in SWHs but is proposed for other working fluid applications more generally.

■ ASSOCIATED CONTENT

Supporting Information

Additional tables (PDF). This material is available free of charge via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

■ NOMENCLATURE

C	Cost ($ J^{-1})
CHF	Critical heat flux (W)
D	Diameter (m)
G	Solar insolation (W m^{-1})
GA	Genetic algorithm
h	Height (m)
h_{fg}	Latent heat (J kg^{-1})
HP	Heat pipe
k	Thermal conductivity (W m^{-1} C^{-1})
L	Length (m)
M	Mass (kg)
N	Total number of ...
NRTL	Nonrandom two-liquid model
obj	Objective function ($ or dimensionless)
Property	Thermophysical property
PS	Pattern search algorithm
Q	Heat (W)
SA	Simulated annealing algorithm
SWH	Solar water heater
T	Temperature (C)
TD	Temperature-dependent mode
TiD	Temperature-independent mode
x	Composition

Greek Symbol

σ	Surface tension (N m)
2υ	Groove wall inclination angle (deg)
μ	Viscosity (Pa s)
ω_2	Groove base width (m)
ρ	Density (kg m^{-3}

Subscripts and Superscripts

a	adiabatic section/air/ambient
c	condenser section
con.pipes	connecting pipes
e	evaporator section
f	circulating fluid
g	cover glass/groove
i	inner/counter/component ID
in	inlet
ins.	insulation
mani	manifold
mix	Working fluid mixture
N	Nth
o	outer
opt	optimum
t	tank
tot	total
ν	vapor

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