OPTIMIZATION OF THE C3MR CYCLE WITH GENETIC ALGORITHM

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ABSTRACT

The aim of this paper is thermodynamic simulation and optimization of the C3MR system with Genetic Algorithm. For this purpose, in the first step, the Peng Robinson equation of state is simulated with a code in MATLAB and then used for simulating thermodynamic properties of natural gas and refrigerants that are used in the cycle. Following that the cycle is thermodynamically simulated and composite curves for subcooling and liquefaction heat exchangers are plotted. If composite curves in heat exchangers approach, the total power will decrease. Then, the total power used by the compressors is calculated. In the next step, the thermodynamic modeling is linked with Genetic Algorithm and the total power consumed by compressors is defined as objective function. The best value resulted from optimization has 23% lower power than the base design. In addition, heat exchange curves closed together.

Keywords: LNG; Optimization; C3MR; Genetic Algorithm.

OPTIMISATION DU CYCLE C3MR PAR LE MOYEN D'ALGORITHMES GÉNÉTIQUES

RÉSUMÉ

Cet article s'intéresse à la simulation et l'optimisation d'un système par le moyen d'algorithmes génétiques. Pour arriver à notre objectif, nous simulons la première équation d'état de Peng Robinson à l'aide d'un code dans MATLAB, et ensuite nous l'utilisons pour la simulation des propriétés thermodynamiques de gaz naturel et de réfrigérants qui sont utilisés pendant le cycle. Par la suite, le cycle est simulé, et les courbes composites pour la surfusion et la liquéfaction des échangeurs de chaleur sont définies. Si des courbes composites dans les échangeurs de chaleur s'approchent, la valeur de la puissance totale diminuera. Ainsi la puissance totale utilisée par les compresseurs est calculée. Dans l'étape suivante, le modèle thermodynamique est relié par des algorithmes génétiques et la puissance totale consommée par les compresseurs est définie comme fonction objective. Le résultat de la valeur optimale de l'optimisation est de 23% moindre que dans la conception de base.

Mots-clés: LNG; optimisation; C3MR; algorithmes génétiques.

Nomenclature

a	attraction parameter (MPam^6 kmol^{-2})
b	molecular co-volume parameter (m^3 kmol^{-1})
h	specific enthalpy (J/kg)
k	binary interaction parameter
$\dot{m}$	mass flow rate (kg/s)
p	pressure (MPa)
Q	heat transfer, W
R	universal gas constant (8.314 × −10^{-3} MPam^3 kmol^{-1} K^{-1})
T	temperature (K)
v	volume (m^3 kmol^{-1})
W	net power output, W
x	liquid phase composition (also phase composition)
y	vapour phase composition

Greek symbols

ω	acentric factor
f	partial fugacity coefficient

Subscripts

c	critical
i,j	components i and j
i	input
o	output
MR1	mixed refrigerant is used in liquefaction
MR2	mixed refrigerant is used in subcooling process

Superscripts

V	vapour
l	liquid

1. INTRODUCTION

The use of energy resources with less or no influence on air pollution and environment is required and the rational use of available energy is recommended [1,2]. Liquefied natural gas (LNG) is known as a clean energy source that is commonly used as domestic and industrial fuel for combustion. LNG is composed of 85–99% methane by mole fraction, a few percent ethane, and propane depending on its production site. Since moisture and sulphur are contained in crude natural gases, they should be removed during the liquefying pre-process. Natural gas is widely used in electricity generation and daily living for its friendly environmental performance [3].

Since the first LNG trade in 1964, the global LNG trade has observed a continuously rapid growth, mainly because the transformation from natural gas to the LNG reduces its volume by about 600-fold and thus facilitates the transfer conveyance from the gas source to receiving terminal. During the liquefying process, a large amount of mechanical energy is consumed in refrigeration process, approximately 500 kWh electric energy per ton LNG; so LNG contains a considerable portion of the energy and exergy invested in this process (cryogenic energy) [4].

Studies on the operation of complex vapor compression cycles, like the one used for the production of LNG, are not widely reported in the open literature [5]. Most low temperature processes feature one or more refrigeration cycles with the purpose of removing heat from subambient hot streams. The provision of a cryogenic cooling requires significant power demands for compression and it is very important to achieve high-energy efficiency in the design and operation of refrigeration cycles, leading to low carbon emissions into the environment. In a simple system with a closed refrigeration cycle, the heat is removed by vaporization of a low-pressure refrigerant, which is then compressed and condensed at a higher pressure against a warmer cold utility or heat sink. The condensed liquid is let down in pressure (and temperature) by means of an expanding device such as a throttle valve. When cooling for a wide temperature range is required, a complex arrangement (for example, a cascade cycle or a cycle with multilevel cooling) is introduced to improve thermodynamic efficiency of the refrigeration systems [6]. On the other hand, using Mixed Refrigerant (MR) in the refrigeration cycles provides very promising potential to yield more efficient, yet simple and reliable systems in comparison to pure refrigerant ones because a mixture of refrigerants is evaporated isobarically, not at a single but in a range of temperatures. Although there are important "natural" applications for MR cycles (e.g., LNG), their optimal design has not been the object of extensive research as in the case of pure refrigerant systems [6].

A liquefaction process of natural gas has been optimized in peak shaving plant using Genetic Algorithm (GA) [7]. However, peak shaving plants had a relatively low load and used in special seasons in year. The aim of this paper is the thermodynamic simulation and optimization of the C3MR system with GA. For reaching this goal, first Peng Robinson equation of state is simulated. Then, it was used for simulating the properties of natural gas and the refrigerants that are used in the cycle. Then, the cycle is thermodynamically simulated and composite curves for subcooling and liquefaction heat exchangers and the total power used by the compressors are calculated. Then, the thermodynamic modeling is linked with Genetic Algorithm. The optimization algorithm is explained. The constraint of 3°C is applied for the minimum distance between hot and cold composite curves.

2. MR SYSTEMS

Increasing concerns about greenhouse effects on climate and ecological problem by certain chlorofluorocarbon (CFC)-based refrigerants, have forced the refrigeration-based industries to direct the research trends in search of alternative refrigerants and alternative technologies [8]. Using mixed refrigerants is a choice to replace the environmentally harmful CFCs [9]. Achievement of high energy efficiency in MR systems have been shown [9,10].

A MR system uses a mixture as the refrigerant rather than several pure refrigerants as in conventional multistage or cascading refrigeration systems [12]. In contrast to pure refrigerants, mixed refrigerants evaporate and condense in a range of temperature at a constant pressure. The composition of the mixture is selected such that the liquid refrigerant evaporates over a temperature range similar to that of the process cooling demand. A mixture of hydrocarbons (usually in the C1-C4 range) and nitrogen (because of its low critical temperature) is usually used to achieve the desired refrigerant characteristics in natural gas liquefaction (e.g., close matching of the hot and cold composite curves, with small temperature driving forces over the whole temperature range) for the specific refrigeration demand. If the temperature driving forces are very small, then the operation will approach a reversible operation, a higher thermodynamic efficiency, and a lower power requirement. In addition, a MR system, unlike pure cascade cycles, has a simpler machinery configuration and fewer maintenance problems. Several variations and applications of mixed-component refrigerant have been introduced [12–14]. Some references showed that MR systems have more efficiency than turbo-expander systems in natural gas liquid (NGL) recovery processes [15]. Duvedi et al. [16] used a mixed-integer nonlinear programming approach for the design of refrigerant mixtures that have the desired attributes. However, the approach was limited to a small number of refrigerant components, and the assumptions made in the MINLP model were far from realistic. In the design of MR systems, we need to be concerned not only about the minimization of energy and capital costs, but also about the temperature profiles of the evaporation and condensation processes. Usually, the temperature approach within the heat exchangers of MR systems is as small as 1°C to 3°C.

3. MODELING

The simplified diagram of the C_3MR cycle is shown in Fig. 1. The cycle is composed of three subcycles. The first is the precooling process in which Crude Gas (133–134) and MR_1 (221–222) and MR_2 (233–234) refrigerant are precooled. The refrigerant of the subsycyle is Propane. In the second subcycle, i.e., liquefaction process, Crude Gas (134–135) is liquefied and the MR_2 (234–235) is precooled again. Finally, in third subcycle, i.e., the subcooling process Crude Gas is subcooled and exit as LNG (136–137). MR_1 is composed of Methane, Ethane, and Propane and MR_2 is composed of Methane, Ethane, and Nitrogen. In this paper, the C_3MR cycle is thermodynamically modeled and then simulated by a code in MATLAB software.

One major step in the thermodynamic modeling is simulating of material properties. For thermodynamic properties simulation, various methods are proposed. Many researchers have studied equation of state (EoS) for refrigerant mixtures [17, 18]. However, they are not widely used and their correctness is not verified. One of the best-improved equations of states is Peng-Robinson EoS [19] and many researchers have studied and improved it. In this paper, this EoS has been used.

$$P = \frac{RT}{v-b} - \frac{a(T)}{v(v+b)+b(v-b)}, \tag{1}$$

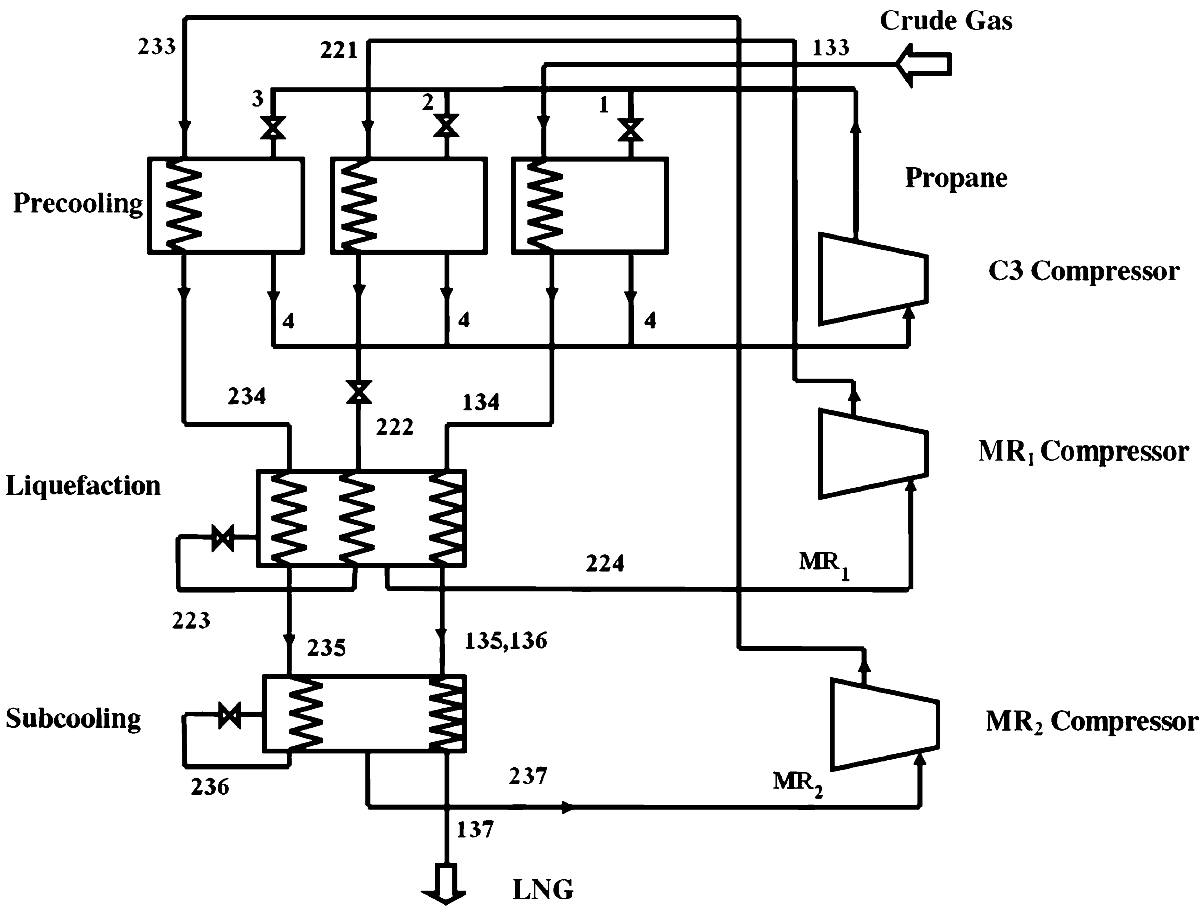

Fig. 1. Simplified diagram of the C3MR cycle.

$$a(T_c)=0.45724\frac{R^2T^2}{P_c}, \tag{2}$$

$$b(T_c)=0.07780\frac{RT_c}{P_c}, \tag{3}$$

$$a(T)=a(T_c).\alpha(T_r,\omega), \tag{4}$$

$$b(T_c)=b(T_c), \tag{5}$$

Where $\alpha(T_r,\omega)$is a dimensionless function of reduced temperature and acentric factor and equals unity at the critical temperature.

$$a^{1/2}=1+\kappa\left(1-{T_r}^{1/2}\right), \tag{6}$$

$$\kappa=0.37464+1.54226\omega-0.26992\omega^2, \tag{7}$$

The mixture equilibrium calculations can be carried out by solving the following simultaneous equations:

$$T^l=T^v, \tag{8}$$

$$P^l=P^v, \tag{9}$$

$$xi\varphi_i^l=yi\varphi_i^v, \tag{10}$$

The fugacity coefficients are calculated using the Peng-Robinson EoS equation. The system is assumed to operate at steady state and the refrigerant flow leaving one component is same conditions as the one entering the next one. The kinetic and potential energies are negligible and thus they are not considered. The system is adiabatic and thus the heat is only exchanged by heat exchangers. In addition, it is supposed that natural gas has a constant mixture through the cycle. The throttling process is supposed to be adiabatic so the inlet total enthalpy is equal with the exit one. The pressure drop in the heat exchangers was assumed zero.

For the thermodynamic analysis of the system, the principles of mass conservation, the first and the second laws of thermodynamics are applied to each components of the system in a similar manner used by Lee [20]. Each component can be treated as a control volume with inlet and outlet streams and heat transfer and power interactions. In the system, mass conservation includes the mass balance of total mass and each material of the solution.

Table 1. An example of mass flow rate.

$\dot{m}_{MR1}$	$\dot{m}_{MR2}$	$\dot{m}_3$	$\dot{m}_2$	$\dot{m}_1$
655190	1383994	528042	835479	490872

The governing equation of mass conservation for a steady state and steady flow system is:

$$\sum \dot{m}_i - \sum \dot{m}_o = 0 \tag{11}$$

The first law of thermodynamics yields the energy balance of each component of the system as follows:

$$\sum (\dot{m}h)_i - \sum (\dot{m}h)_o + \left[\sum Q_i - \sum Q_o\right] + W = 0 \tag{12}$$

The above equation yields the energy balance of each component (each component can be treated as a control volume with inlet and outlet streams, heat transfer and power interactions) of the system.

4. VALIDATION

Considering the mentioned assumptions, the system was modeled with a code in MATLAB®. For confidence from the correctness of the code, we modeled the cycle in the Hysys® software [21] at the same condition and then compared their results. For this purpose, the conditions in Tables 1 and 2 are taken into account.

After running the code and Hysys® software, we got the results shown in Figs. 2–5. In this step the total power that was calculated by the code is nearly 196 Mw.

In Fig. 2, the refrigerant curve has a breakage point at $-50°C$. Refrigerant (MR1) is two phase from Q=0 to this point. After this breakage, the refrigerant is single phase. Moreover, the hot stream curve (Δ) is the sum of the heat that exchanged from refrigerant to other streams in this heat exchanger. In the breakage point, the distance between two curves is maximized. There is no temperature cross in this heat exchange process and this shows that the heat exchanger is designed properly. However, the distance between refrigerant curve and the total hot stream curve is high and according to the second law of thermodynamic, it has an extra exergy loss.

Explanations for Fig. 3 are the same as Fig. 2. It seems that the heat exchange curves are close here and this shows that the design of this heat exchanger is better than the former. In addition, the breakage point can be observed in this curve too.

Table 2. An example of mole fraction compositions.

Fluid \ Refrigerant	subcooling	MR_1	MR_2
Methane	-	10%	60%
Ethane	-	70%	35%
Propane	100%	20%	-
Nitrogen	-	-	5%

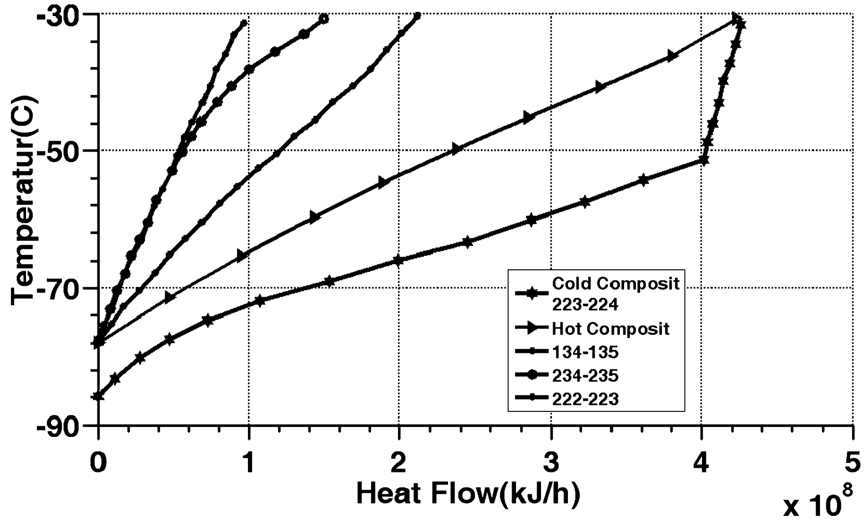

Fig. 2. Composite curves for the liquefaction heat exchanger calculated by the code before optimization.

As it can be seen, the result of the code and Hysys® software are nearly the same. For comparison of the distance between composite curves, we can integrate the area between the hot and the cold composite curves as Eq. (13)

$$A=\sum_{i}\frac{(h(i)+h(i-1))(T(i)-T(i-1))}{2}-\sum_{j}\frac{(C(j)+C(j-1))(T(j)-T(j-1))}{2} \tag{13}$$

.

From Table 3, it can be seen that the result of Hysys® and the code are nearly the same.

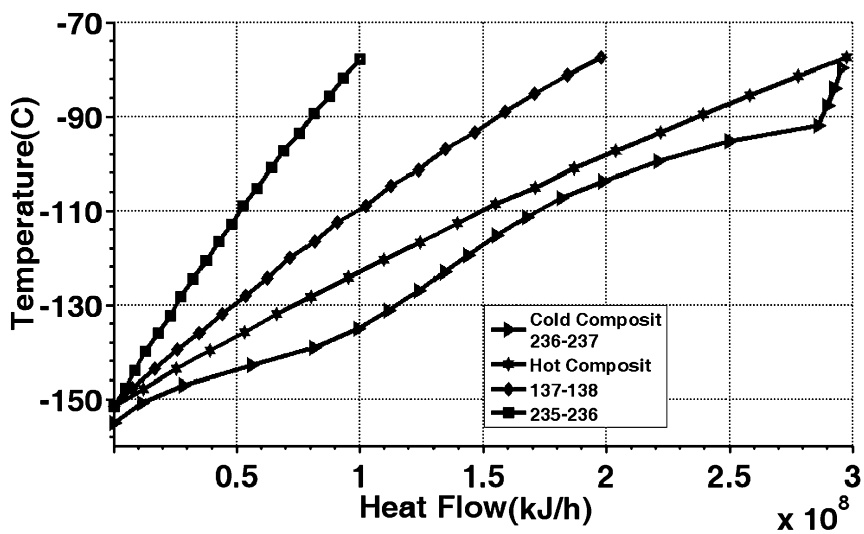

Fig. 3. Composite curves for the subcooling heat exchanger calculated by the code before optimization.

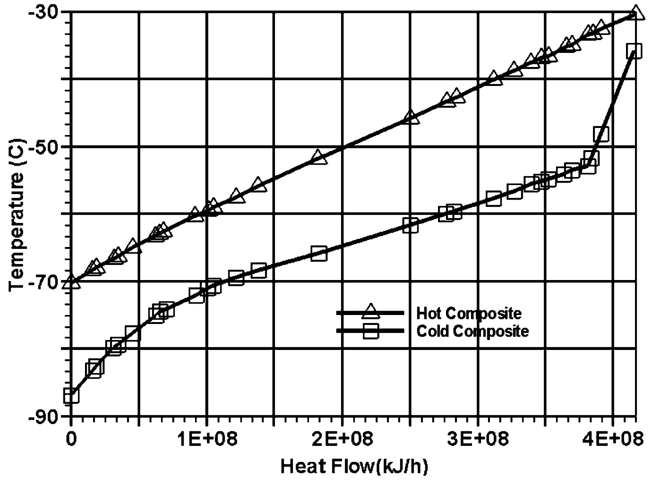

Fig. 4. Composite curves for liquefaction heat exchanger calculated by Hysys® before optimization.

5. MODELING THE PROBLEM AND GENETIC-BASED OPTIMIZATION

For optimization, first the total power used by the compressors of the cycle is defined as the objective function. In addition, the goal is to minimize this function. The 11 unknown variables are listed in Table 1 and Table 2. The optimization problem is of the NLP type and not all the formulation has been explicit (e.g., phase equilibrium and physical property calculations).

There are many calculus-based methods including gradient approaches to search for mostly local optimum solutions and these are well documented in the literature [22, 23]. However, some basic difficulties in the gradient methods such as their strong dependence on the initial guess can cause them to obtain a local optimum rather than a global one. This has led to other heuristic optimization methods, particularly genetic algorithms (GAs) being used extensively during the last decade. Genetic algorithms [24, 25] are highly robust and efficient search and optimization methods; they draw inspiration from natural selection and evolution for finding the global

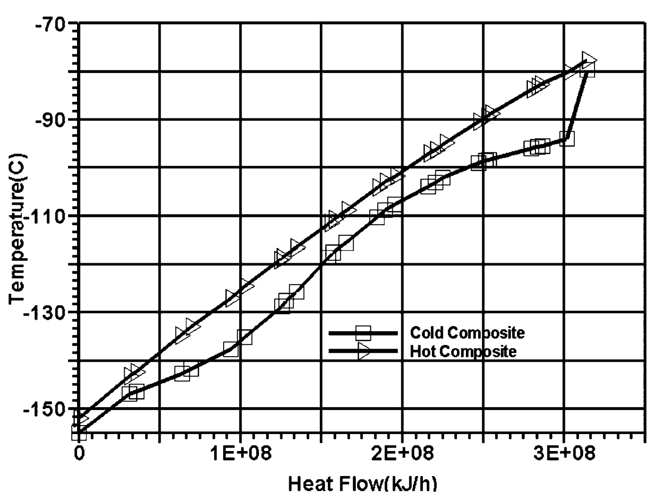

Fig. 5. Composite curves for the subcooling heat exchanger calculated by Hysys® before optimization.

Table 3. The integration results.

Fig.	A(kJ/h°C/10^8)
2	1.1101
3	0.3296
4	1.5493
5	0.6334

optimum. They have been applied to various scientific disciplines including materials science for alloy microstructure and process optimization [26–30].

The evolution starts from a population of randomly generated chromosomes and happens in generations. In each generation, every individual is evaluated by measuring its fitness function (total power used by compressors) in the population and assigning a score to it. Based upon their fitness, multiple individuals are stochastically selected from the current population to form the next population of n=2 individuals. To create the next generation, new individuals, called offspring, are formed by either merging two chromosomes from the current generation using a crossover operator or modifying a chromosome using a mutation operator. The crossover operator takes two selected individuals and combines them about a crossover point thereby creating two new individuals. The mutation operator randomly modifies the genes of a chromosome, introducing further randomness into the population. The cycle restarts by the formulation of a new generation by selection and according to the fitness values, some of the best parents and offspring are kept whereas the others are rejected to keep the population size constant. The algorithm ends when either a maximum number of generations have been produced or a satisfactory fitness level has been reached.

5.1 Optimization Problems

The main problem in optimization is the temperature cross. This violates the second law of thermodynamics. Consider Table 1 as the inputs for mass flows and Table 4 for mixtures. The simulation result for subcooling heat exchanger is shown in Fig. 6.

It can be seen from Fig. 7 that the temperature cross occurs at near −150 °C. As it was mentioned this violates second law of thermodynamics. As we like to minimize the exergy loss in the heat exchangers, the distance between two cures should be minimized. But according to Eq. 14 with a known U and Q when the ΔT_m decreases A increases and this increases the cost.

$$Q = UA\Delta T_m \tag{14}$$

According to this equation, if ΔT_m limits to zero, then A will limit to infinity. But in practice this cannot happen. For overcoming this problem, some studies have proposed a minimum

Table 4. Refrigerant compositions for a sample temperature cross.

Refrigerant / Fluid	subcooling	MR_1	MR_2
Methane	-	10%	60%
Ethane	-	70%	39.5%
Propane	100%	20%	-
Nitrogen	-	-	0.5%

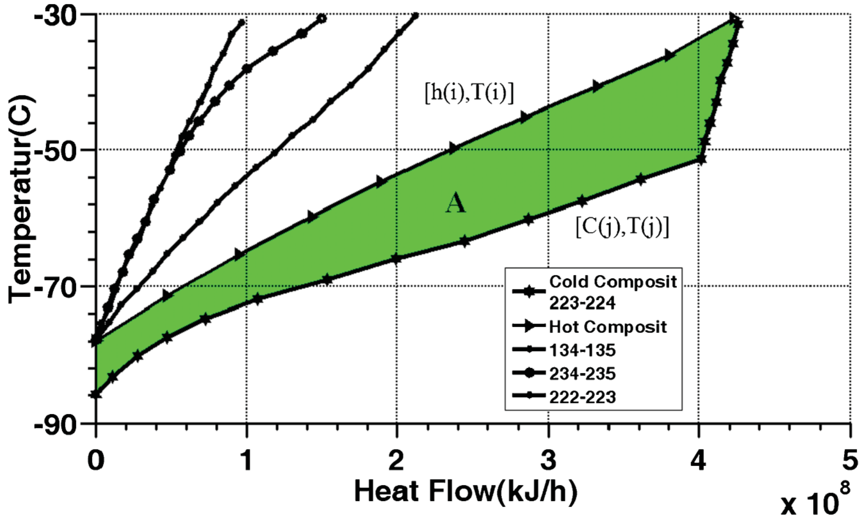

Fig. 6. Example for calculation of the area between hot and cold composite curves.

temperature difference for example 3°C [16]. We follow this procedure and define the minimum temperature difference of 3°C as a constraint for genetic algorithm. As it was mentioned, the goal is minimization of total power. For this purpose, each member of the population in the genetic algorithm must satisfy the following constraints:

1. The total heat exchange curves must not cross.
2. After satisfying first constraint, the minimum temperature difference between total heat exchange curves must be more than 3°C.

Some individuals do not satisfy the first constraint, for example like the one shown in Fig. 7. For the second constraint, consider Table 5 as a population. The simulation result for the liquefaction and subcooling heat exchangers are shown in Figs. 8 and 9.

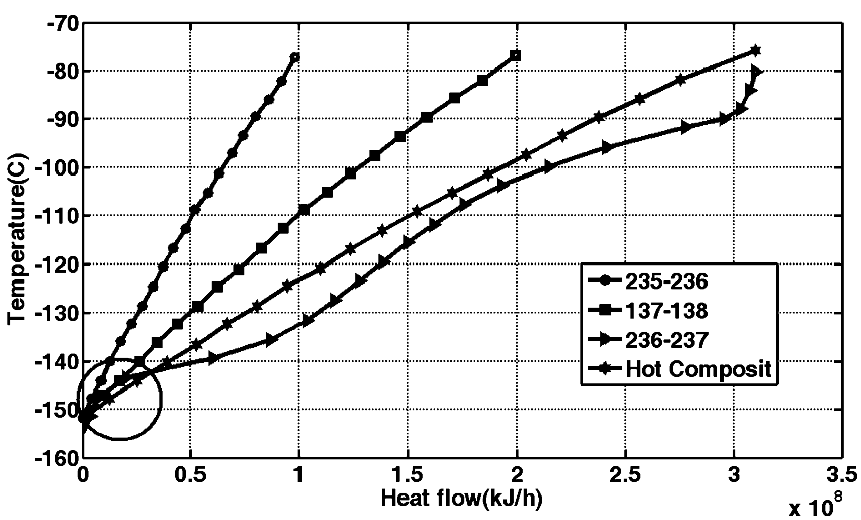

Fig. 7. Composite curves for a sample temperature cross.

Table 5. Input mass flow rate for an individual that does not satisfy first constraint.

$\dot{m}_{MR_2}$	$\dot{m}_{MR_1}$	$\dot{m}_3$	$\dot{m}_2$	$\dot{m}_1$
487886	945165	528042	1383994	655190

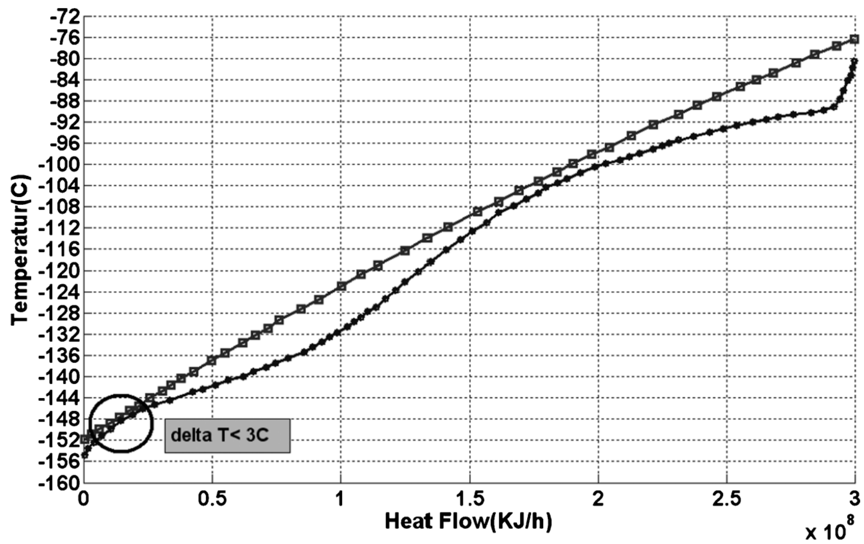

Fig. 8. Composite curves for an individual that does not satisfy the second constraint in liquefaction process.

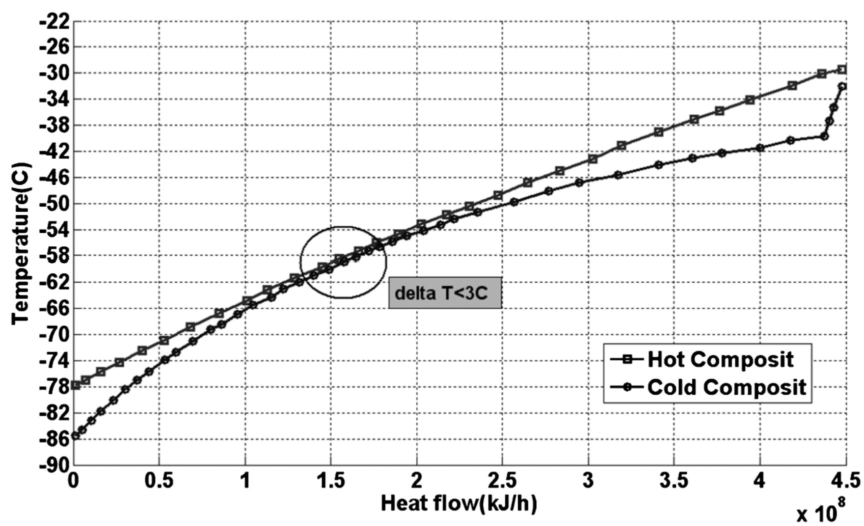

Fig. 9. Composite curves for an individual that does not satisfy the second constraint in subcooling process.

6. RESULTS AND DISCUSSION

As has been mentioned, a single objective genetic algorithm is used for optimization of the system. In the present study, tournament selection, uniform crossover, and one-point mutation were selected. The best parent is reproduced (copied) into the new population. After the new

Table 6. Refrigerant composition for an individual that does not satisfy second constraint.

Fluid \ Refrigerant	subcooling	MR_1	MR_2
Methane	-	30.3%	57.4%
Ethane	-	26.2%	41.4%
Propane	100%	43.5%	-
Nitrogen	-	-	1.2%

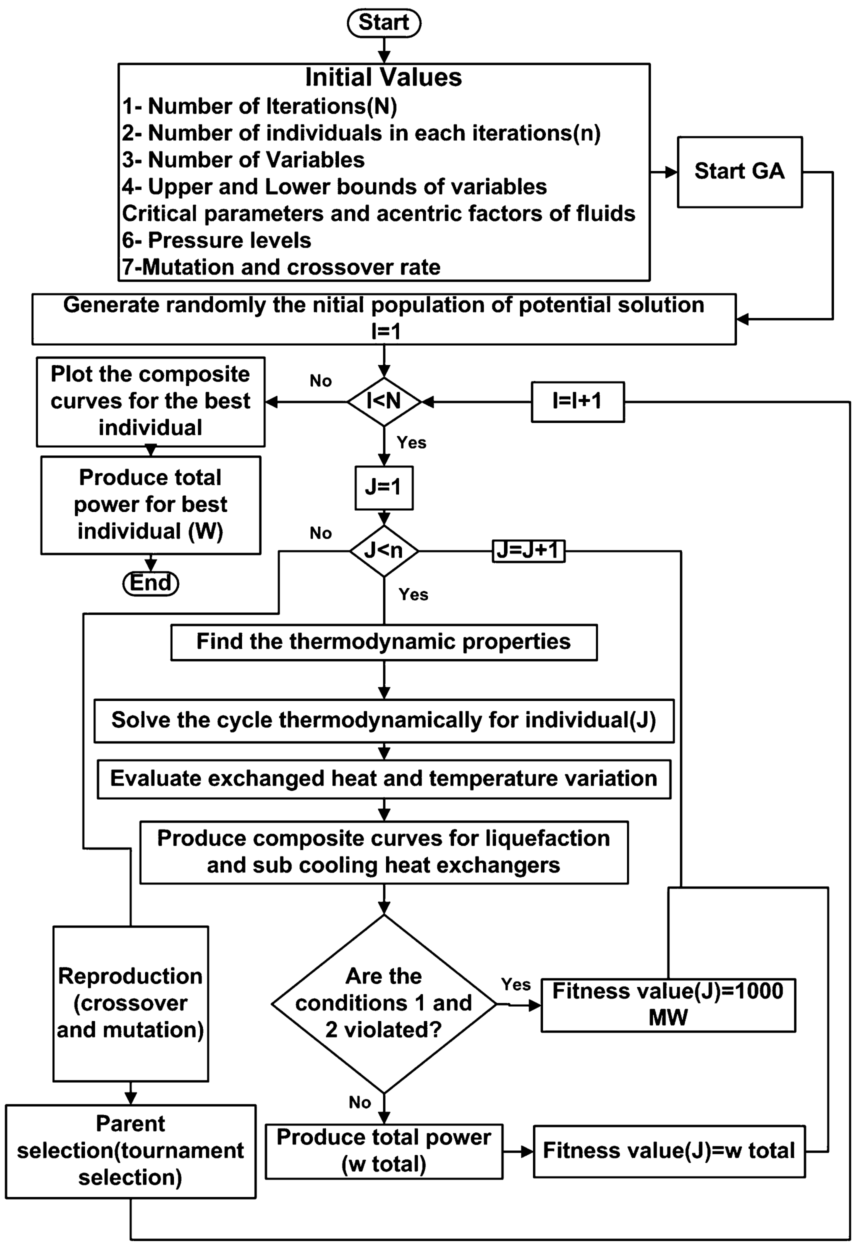

Fig. 10. The algorithm of optimization process.

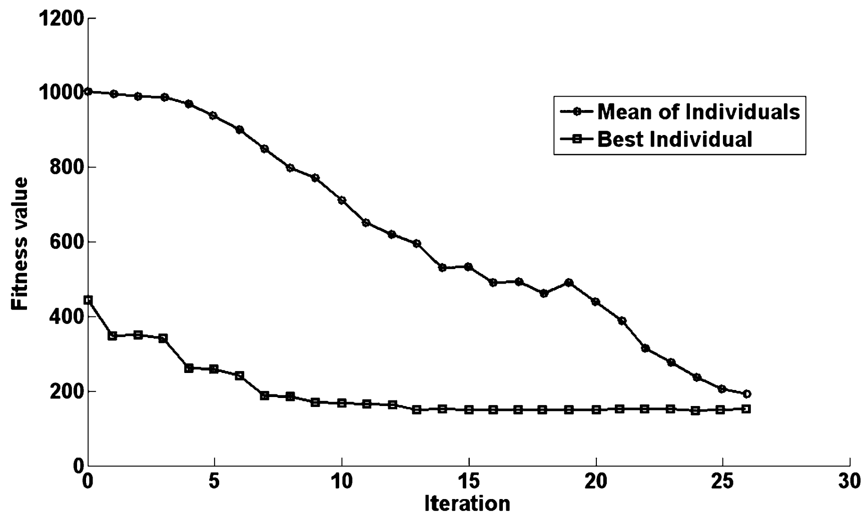

Fig. 11. Optimization process by GA for 1000 individuals.

population is generated, GA checks if the best parent has been replicated. The size of population and maximum evolution generation are set to 1000 and 30, respectively. Probability of crossover and mutation are set to 0.5 and 0.005, respectively.

The first and second constraints (that is specified in Section 5.1) are not predictable so it cannot be defined as a constraint beforehand in the optimization process. A solution for this problem is, if the constraints are not satisfied, then the objective function should be replaced by a big value; therefore with evaluating the genetic algorithm the bad individuals will disappear and finally the best individual is found as the optimal value of their objective function. Maybe none of the individuals satisfies the two constraints in the initial steps. But in the evaluating process, the individuals that satisfy these constraints are produced and the bad individuals are omitted. The algorithm of optimization process is shown in Fig. 10. We substituted 1000 MW for bad individuals.

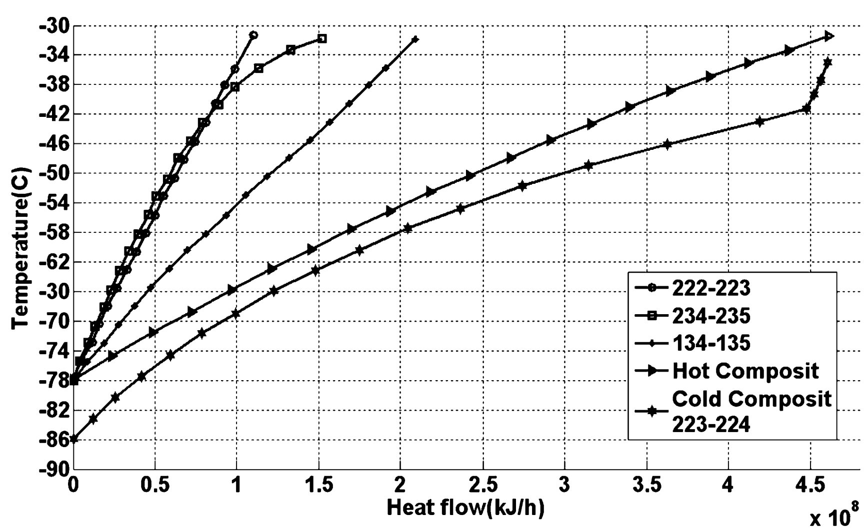

Fig. 12. Composite curves in the liquefaction process for the best individual.

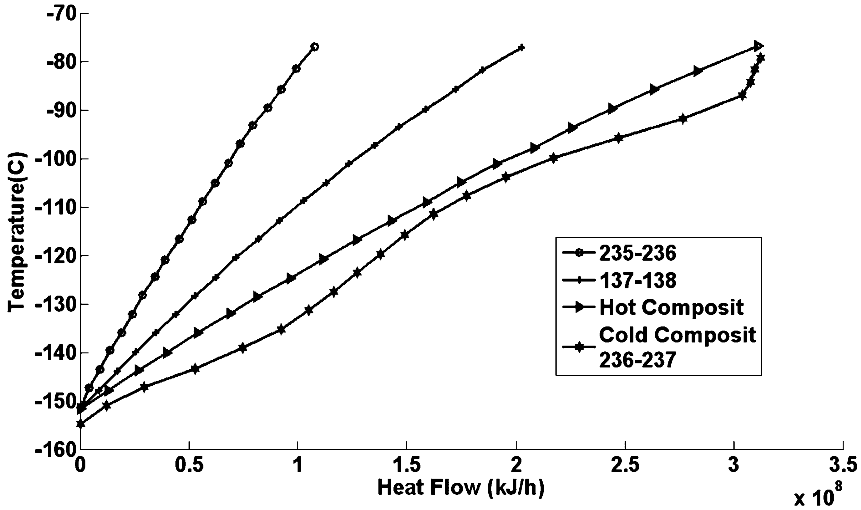

Fig. 13. Composite curves in the subcooling process for the best individual.

The optimization process is shown in Fig. 11. In this figure, the upper curve shows the mean value for all individuals and the lower one shows the best individual value in each step. It can be seen that the mean value for all individuals in the initial steps are nearly 1000 MW. It shows that all individuals in the first steps are bad, but gradually the good individuals are produced and the mean value decreases and in the final step, all individuals are the same and the algorithm stops.

Figures 12 and 13 show the temperature profiles and the temperature approach in the heat exchanger, respectively. The minimum temperature approach occurs at the warm end.

The optimization procedure has been run many times, but the results were the same with Fig. 10. The optimization values of unknowns are summarized in Tables 7 and 8.

Again, the area between the hot and cold composite for Figs. 12 and 13 was calculated and presented in the Table 9.

Table 7. Optimization result for refrigerant compositions.

$\dot{m}_{MR_2}$	$\dot{m}_{MR_1}$	$\dot{m}_3$	$\dot{m}_2$	$\dot{m}_1$
535131	978124	519031	1182500	646100

Table 8. Optimization result for refrigerants compositions.

Refrigerant / Fluid	subcooling	MR_1	MR_2
Methane	-	20.9%	55.5%
Ethane	-	34%	42.3%
Propane	100%	45.1%	-
Nitrogen	-	-	2.2%

Table 9. The area between the hot and cold composite for Figs. 12 and 13.

Fig.	A(kJ/h°C/10^8)
10	0.2192
11	0.2513

By comparing Tables 8 and 9, it can be seen that the area between cold and hot composite for liquefaction and subcooling heat exchangers decreased in the optimization process. Moreover, this shows that the hot and composite curves get close. When two curves approach, the heat exchange process becomes more reversible and this event influences the total function of the cycle. The result of Genetic Algorithm is shown in Fig. 11 and the total power decreased to 149 MW, i.e., the total power is decreased by nearly 23%.

7. CONCLUSIONS

In this paper, a C3MR system was studied. First, the system was thermodynamically modeled in MATLAB software. The modeled system was linked with a GA code in the software. Heat exchangers composite curves were a good concept for optimization. It was then tried to make composite curves get closed. Composite curves crossed in sometimes. According to literature, a minimum margin of 3°C is used for optimization. This has been defined as a constraint for GA. Chromosomes were generated randomly and the fitness functions for the Chromosomes that could not satisfy the margin of 3°C, were replaced with 1000 MW. After 26 generations, the best value did not change and the minimum power and the best individuals were obtained. The best value obtained from optimization had 23% lower power than the base design.

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