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Genetic-algorithm-based fault detection of the heat transfer process in nuclear-based hydrogen production based ON Cu–Cl cycle

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ABSTRACT

In the heat transfer process of nuclear hydrogen production system based on a 4-step Cu–Cl cycle, there are three major varying temperatures, namely room temperature, hydrolysis temperature and oxygen decomposition temperature. The heat requirement of the system will change with the temperatures. Therefore, it is important to identify the optimal ranges of the varying temperatures to make sure the heat requirement will be satisfied by the heat from a nuclear power plant, when the temperatures fluctuating in the optimal ranges. Genetic-algorithm-based Monte Carlo simulation method is developed in this paper to identify the optimal ranges. This method is able to obtain the optimal ranges through random sampling. The final result indicates that GA-based MCS method can be applied to identify the optimal ranges of the varying temperatures in the heat transfer process, and the ranges are highly trustable.

Introduction

Fossil fuels as a type of non-renewable resource are widely used all over the world nowadays. With increasing consumption of them, the reserves are diminishing and will be exhausted in a not far future. Moreover, burning such resources will generate pollutant source such as CO_2 which is known as greenhouse gas and cause average temperature increasing of the earth's surface. On the other hand, as a sustainable and greenhouse-gas-free resource, hydrogen is expected to resolve this urgent energy crisis, therefore attracts growing interests from many countries recently.

Many industrial ways to produce hydrogen have been researched, such as steam electrolysis, biomass method and radiolysis of water. Among all of these methods, copper-chlorine cycle (Cu–Cl cycle) was found to be a promising way to achieve large-scale production of hydrogen due to its lower temperature requirement and lower cost. A collaborative effort has taken place by Argonne National Laboratories (ANL), Atomic Energy of Canada Limited (AECL), University of Ontario Institute of Technology (UOIT) and other partners to design the Cu–Cl thermochemical cycle for hydrogen production, starting in September of 2010 [1].

In the Cu–Cl cycle, water is decomposed into hydrogen and oxygen through intermediate copper and chlorine compounds

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with the highest heat temperature input requirement of 530 °C [20]. The relatively low temperature requirement allows the cycle to utilize waste heat of nuclear power plant in a wide range. Other than this advantage, lower demands on materials of equipment, none solid product and minimal cost for raw material also illustrate that the Cu–Cl cycle is of high potential to become a promising method for mass hydrogen production.

As a recently-built system, nuclear-based hydrogen production system is still under developed in CERL and needs more experiments to put it into use. Fault identification is an essential process among all the tests and experiments need to be done, since people need to rule out the possibility of accidents happening caused by potential hazards before operating. For example, insufficient heat from NPP will result in incomplete reactions in hydrogen production system, or even ceasing operation. In addition, many uncertainties, such as fluctuating room temperature, will cause the change in heat requirement which also necessitate fault identification. However, since the target system is a new type of system, the major obstruct of doing fault identification is lacking data and expert experience. Moreover, for water-splitting technology used in nuclear-based hydrogen production, the process can only be completed when there is enough amount of heat from the nuclear plant [3]. Hence, the main purpose of this paper is to find out that with only sparse data provided, the optimal ranges of the varying temperatures to make sure the heat requirement will be satisfied by the heat from a nuclear power plant when the temperatures fluctuating in the optimal ranges, in other words, to optimize the given ranges of the varying temperatures.

For heat transfer process, there are three major barriers for doing such optimization. The first is highly nonlinear, since the heat transfer process contains various heat transfer points, at which there are different transfer equations which are of high complexity. The second is multiple variables under different constraints. Because at each heat transfer point, there exists uncertainty in certain temperatures, like the room temperature which will fluctuate in a given range and cannot be controlled. The third is large searching space. In order to gain a more accurate result, the searching space should be large enough to get a global minimum/maximum value.

A useful optimization method should not only be able to deal with the three challenges, but also achieve high accuracy and fast convergence. During the 1950s, some computer scientists were inspired by biological evolution and first proposed the concept of evolutionary algorithm which was applied as an optimization technology to solve engineering and searching problems. The competence of these algorithms can depend on the fact that they imitate the best features in nature, especially the selection of the fittest in biological systems which have evolved by natural selection over millions of years [4].

The last two decades have seen enormous development in use of metaheuristics in many science fields including artificial intelligence, computational intelligence, soft computing, mathematical programming, and operations research [4]. Among them, Particle Swarm Optimization (PSO) was first proposed by Eberhart and Kennedy [6] in 1995, it is a population based stochastic global optimization technique evolved to study the social behavior of insects, birds or fish as why they move in a group searching for food randomly in some area, knowing only the distance from the food [7]. It is capable of solving difficult nonlinear and multi-dimension problems, and insensitive to the scale of searching space. However, parameters of it need to be taken good care of, otherwise, the result can be less accurate. Ant Colony Optimization (ACO) is another evolutionary method [8], it is an agent-based system, which simulates the natural behavior of ants and develops mechanisms of cooperation and learning [9]. It was first proposed in 1992 by Dr. Dorigo in his PhD thesis to numerical optimization problems. Fast and mature convergence can be guaranteed by AC, but it has inherent disability to deal with continuous problems. Other methods like Artificial Bee Colony (ABC) [10], Gravitational Search Algorithm (GSA) [11], and Cuckoo Search (CS) [12] et al. are all evolutionary algorithms widely utilized to solve complex computational optimization problems in many areas over past decades, limitations like low convergence and unguaranteed accuracy make them inapplicable to the target problem.

An integration of Genetic Algorithm (GA) and Monte Carlo Simulation (MSC) method is applied in this paper to find the ranges of three changing temperatures in heat transfer process. A genetic algorithm is a randomized, population-based search technique that has its roots in the principles of genetics [13]. It has the ability to optimize variables in an extremely complicated space, since it introduces diversity in two steps which help avoid converging to a local minimum/maximum point. On the other hand, MCS is a computational algorithm aims at predicting the result or a trend of a system by sampling randomly and repeatedly. It is capable of dealing with multi-dimensional problems and expand the dataset, so comparing with other methods which can cope with sparse data, like Sparse Principle Component Analysis (Sparse PCA) and Bayesian analysis, it is feasible to the target problem.

In this paper, GA is used to find the optimal solutions for the target problem, and MCS method is applied for performance analysis to evaluate the reliability of the solutions found by GA. They are integrated to deal with the problem raised by varying temperatures. The dataset is expanded through this method, and the final ranges are found based on the expanding dataset that whenever the temperatures drop out of the ranges, the energy provided for the reactions in heat transfer process is not sufficient.

The rest of the paper is organized as follow: in Section Hydrogen production based on Cu–Cl cycle, the heat transfer process of Cu–Cl cycle is generally presented, the heat transfer points are demonstrated in detail. In Section GA-based MCS method, GA-based MCS method is firstly introduced. The process of fault identification is discussed afterwards. The results are found based on the simulation, and confidence interval estimation is presented then to evaluate the reliability of the results. Conclusion is drawn in Section conclusions.

Hydrogen production based on Cu–Cl cycle

Thermochemical cycles are emerging technologies for hydrogen production in recent years. Usually two or more

intermediate chemical compounds are involved and reused internally in the cycles, water will be split into H_2 and O_2 through a sequence of chemical and physical reactions without exhausting any harmful compounds to the external environment. Over the past years, more than 200 thermochemical cycles have been developed by researchers, such as sulfur–iodine (S–I) cycle and calcium-bromine-iron (UT-3) cycle.

There are mainly 3 steps in S–I thermochemical cycle, like other thermochemical cycles, the intermediate compounds are recycled in the reactions. Though it is an economic method to generate hydrogen, the required temperature of this cycle can be over 850 °C which is too high for nuclear hydrogen production. Same as S–I cycle, the main drawback of the UT-3 cycle is that its highest required temperature is around 730 °C [5]. Besides this downside, the UT-3 cycle has a low efficiency comparing to S–I cycle, and the solid products generated in the cycle also need to be tackled with.

The following seven cycles (in addition to the S–I cycle) were identified in a Nuclear Hydrogen Initiative as the most promising cycles: copper-chlorine (Cu–Cl), cerium-chlorine (Ce–Cl), iron-chlorine (Fe–Cl), vanadium-chlorine (V–Cl), copper-sulfate (Cu–SO_4) and hybrid chlorine [2]. Typically, the temperatures required in most of these cycles is more than 800 °C from nuclear power plant reactors which make them unavailable contemporarily. On the other hand, Cu–Cl cycle is more applicable, since the typically required temperature in this cycle is lower than 550 °C. Therefore, it can be connected to the Generation IV Super-Critical Water-cooled Reactor (SCWR).

With the major intermediate chemical compound copper chloride ($CuCl_2$), Cu–Cl cycle splits water into H_2 and O_2 through a sequence of chemical and physical processes, all the chemicals involved in this cycle can be continuously reused in the loop. The schematic of the Cu–Cl cycle is shown in Fig. 1. Since the heat from NPP is directly used in the reactions of the Cu–Cl cycle rather than being transformed into electricity, Cu–Cl is much efficient than traditional hydrogen production method, like water electrolysis. The net efficiency of Cu–Cl cycle is approximately 43%, which is 33% more than electrolysis [15].

There are three types of Cu–Cl cycles which have been developed: 3-step, 4-step and 5-step cycle. In the 5-step cycle, copper is produced in an electrochemical cell, transported to an exothermic hydrogen reactor and then reacted with HCl gas to produce hydrogen gas and molten CuCl (in addition to spray drying and oxygen production steps) [3]. In the 4-step cycle, electrochemical and thermochemical processes are combined in order to avoid the process of handling copper solids. In a 3-step cycle, aqueous $CuCl_2$ is directly transmitted into hydrolysis chamber. This paper focuses on the heat transfer process of the 4-step Cu–Cl cycle, since it was found that the 4-step Cu–Cl cycle has the lowest environmental impact and better thermal efficiency compared to the 3-step and 5-step cycles [16].

The process cycle of a 4-step Cu–Cl cycle is shown below [17,18]:

1. $2CuCl(aq) + 2HCl(aq) \xrightarrow{<100^{\circ}C} 2CuCl_2(aq) + H_2(g)$
2. $CuCl_2(aq) \xrightarrow{90^{\circ}C} CuCl_2(s)$
3. $2CuCl_2 + H_2O \xrightarrow{450^{\circ}C} Cu_2OCl_2 + 2HCl$
4. $Cu_2OCl_2 \xrightarrow{500^{\circ}C} 2CuCl + \frac{1}{2}O_2$

The overall process of 4-step Cu–Cl thermochemical cycle is shown in Fig. 2. The explanation of each step is described as follows:

1. $2CuCl(aq) + 2HCl(aq) \xrightarrow{<100^{\circ}C} 2CuCl_2(aq) + H_2(g)$

This step is electrolysis process, it is achieved by a CuCl/HCl electrochemical cell. Hydrogen is generated through the reaction between copper (Cu) and hydrochloride acid (HCl). Through electrolysis, CuCl solution is decomposed and intermediate product, such as solid copper is generated and sent to be reused.

2. $CuCl_2(aq) \xrightarrow{90^{\circ}C} CuCl_2(s)$

This step includes a drying process, water is vaporized in this step to separate $CuCl_2$ in the solution. This step takes place in a flash dryer at a temperature of 90 °C. Instead of using a flash dryer, the ongoing research at CERL in UOIT is using a new method to pressurize liquid stream in a pressure-reducing nozzle, at a reduced temperature of 70 °C [3].

3. $2CuCl_2 + H_2O \xrightarrow{450^{\circ}C} Cu_2OCl_2 + 2HCl$

This step is hydrolysis process happens in a fluidized bed, solid $CuCl_2$ acquired from step 2 and high-temperature steam (450 °C) will generate HCl which will then be reused in step 1. A large amount of steam is provided in this step to achieve complete reaction and raise the yield of products.

4. $Cu_2OCl_2 \xrightarrow{500^{\circ}C} 2CuCl + \frac{1}{2}O_2$

Oxygen decomposition process takes place in the last step, CuCl yielded in this step will be sent to step 1 for electrolyzing, and oxygen (O_2) which is harmless to the environment will be released. This step requires the highest temperature (over 500 °C) among all steps.

Based on the results of the thermodynamic analysis of the reactions and processes in Ref. [17], the total theoretical heat requirement for the cycle will be 543.8 kJ per mole of H_2O when a 70% heat exchanger effectiveness and a 50% conversion efficiency for heat to electricity is assumed. The Aspen Plus simulation model as shown in Fig. 3 is built based on the layout of Cu–Cl cycle in Fig. 1.

The corresponding heat requirements, input and output temperatures, and other data for the process at each transfer point are shown in Table 1 with 100 mol of water input, 100 mol of hydrogen and 50 mol of oxygen output as the basis.

From Table 1, it can be calculated that with 1 mol H_2 produced the required heat is 517.4 kJ approximately, furthermore, the auxiliary work requires 26.4 kJ based on the simulation, so the total heat requirement for the cycle is 543.8 kJ. The heat transfer points in Table 1 are listed and explained as following: (see Table 2)

Based on the instruction above, all the heat transfer points in Table 1 are classified in terms of reaction steps as following: (see Table 3)

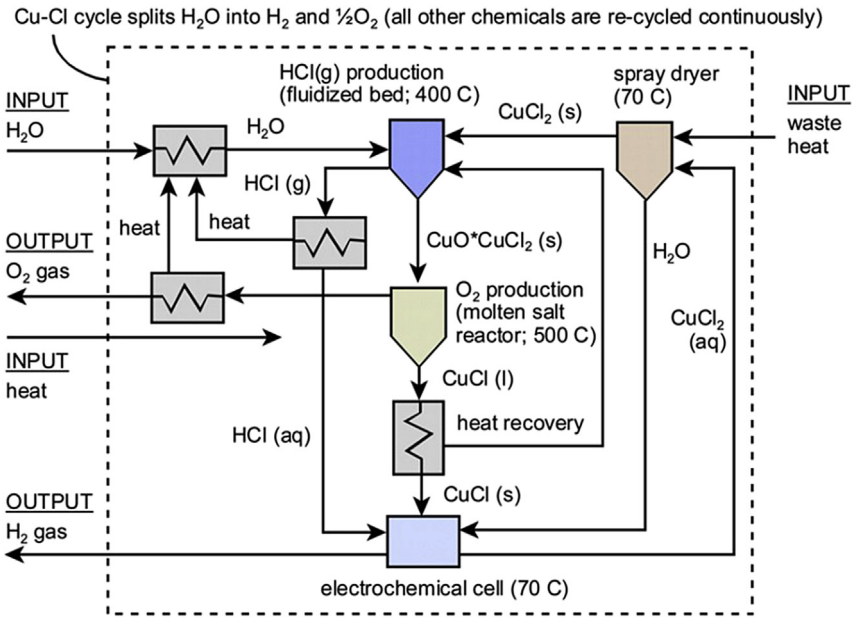

Fig. 1 – Schematic of Cu–Cl cycle [2].

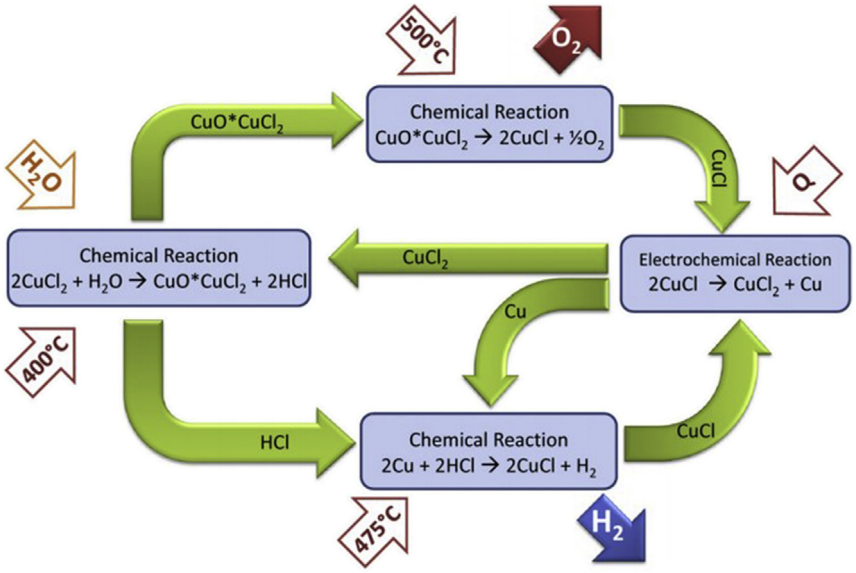

Fig. 2 – The 4-step Cu–Cl cycle [19].

Table 1 shows the simulation result in Aspen Plus, it indicates that some temperatures, like the room temperature, are not fixed as the assigned value. Three temperatures with variation are concerned as major factors which will influence the stability of the reaction. The first is room temperature, almost 50% of the heat transfer points are affected by room temperature. It is assigned 25 °C for the reaction, but since several heaters and coolers are applied in the process, it is not capable to control the room temperature to be a fixed value, it will range from 25 °C to 27 °C as simulation indicates. The second variation is in the reaction temperature of hydrolysis, the assigned temperature is 425 °C, but the simulation result shows this temperature ranges from 425 °C to 450 °C. The last temperature variation is in the process of oxygen decomposition, depending on the simulation result, it will range from 500 °C to 550 °C rather than staying at 550 °C. In conclusion, the overall variation in temperature is shown in Table 4.

Another variation is that, in the heat transfer process, with the temperature changing, the heat capacity of some particular chemical components will also change. For example, CuCl, which is an essential component of the cycle, exhibits allotropy and undergoes phase change within the temperatures of interest in the Cu–Cl cycle [17].

Experiments by Argonne National Laboratory (ANL) [21,22] gave the properties of CuCl at different temperatures by X-ray diffraction, and by Raman spectroscopy, thereby verified the past data from Moscow State University (MSU) [23]. CuCl stays

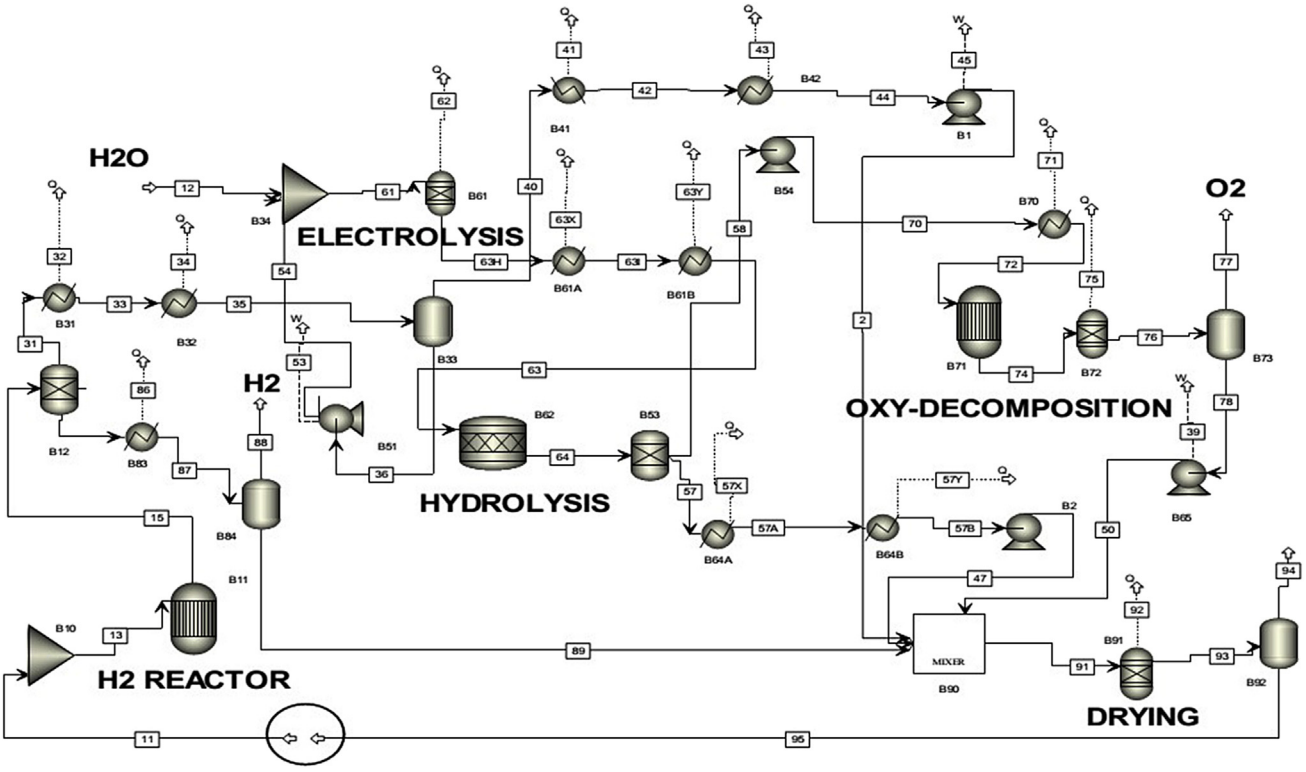

Fig. 3 – Aspen Plus simulation model of four-step Cu–Cl cycle for hydrogen production [17].

in a simple cubic crystalline (SC) form when the temperature is below 685 K, with the temperature increasing, it will melt into liquid (L) when temperature reaches 696 K, and the state in between is called beta-hexagonal (SB). From MSU data, the heat capacity of CuCl can be calculated with the following equations:

$$cp_1(T) = 173.778442133 + 38.206lnx + 0.001298x^{-2} + 0.082339369657x^{-1} + 191.575x \quad (1)$$

$$(x = T \times 10^{-4}; 298.15K < T \leq 685K)$$

$$cp_2(T) = 277.808151505 + 79lnx + 1.3657x^{-1} \quad (2)$$

$$(x = T \times 10^{-4}; 685K < T \leq 696K)$$

$$cp_3(T) = 206.987753087 + 29.319lnx + 0.0583185x^{-2} - 4.11701275112x^{-1} + 74.09 \quad (3)$$

$$(x = T \times 10^{-4}; 696K < T \leq 1200K)$$

Other variation includes solubility of CuCl and $CuCl_2$, and heat capacity of Cu_2OCl_2, but none of them has significant influence on the heat transfer process, so they are not discussed in this paper.

Heat transfer process is essential in Cu–Cl cycle, since it can be executed only when enough heat is provided. From Table 1, the overall heat transferred is 51,734.8 J when 100 mol H_2O is consumed, however, the discussion above shows several variations in the cycle which may result in failure in operation of the system when this amount of energy is provided. Hence, it is important to figure out when this risk will occur.

GA-based MCS method

In this section, GA-based MCS method will first be introduced briefly, and then the process of building fitness function will be presented in detail.

Table 1 – Simulation results for the four-step Cu–Cl cycle.

Heat exchangers	Q (kJ)	T (input) (°C)	T (output) (°C)
32	7494.4	25	100
34	24,409.2	100	116
41	−23,186.0	116	105
43	−2833.6	105	25
57X	−10,736.5	400	90
57Y	32,092.3	90	90
62	−1552.6	113	90
63X	−9697.0	90	27
63Y	55,382.1	27	425
71	559.7	425	550
75	−2718.9	550	25
86	35.1	25	25
92	−17,513.4	117	25
Process heat flow for cycle/100 mol H_2O	51,735.0		

Table 2 – Explanation for all the heat transfer points.

Heat transfer points	Explanation
32	Water is heated up in to steam, from room temperature 25 °C –100 °C.
34	Separating hydrogen from other gases by increasing the temperature from 100 °C to 116 °C.
41&43	Reducing the temperature of the cycle from 116 °C to room temperature.
57X	Recycling $CuCl_2$, temperature drops from 400 °C to 90 °C.
57Y	Drying $CuCl_2$ (from aqueous to solid), temperature remains at 90 °C.
62&63X	Preparing for hydrolysis, separating aqueous and solid $CuCl_2$ up, temperature drops from 113 °C to room temperature.
63Y	Hydrolysis. Heat exchanger provides the required heat for the chemical reaction, temperature increases from room temperature to 425 °C.
71	Oxygen composition. Heat exchanger provides the required heat for the chemical reaction, temperature increases from 425 °C to 550 °C.
75	Recycling and cooling down CuCl to room temperature.
86	Separate the steam, temperature remains at room temperature.
92	Cooling down and recycling HCl, temperature drops from 117 °C to room temperature.

Table 3 – Classification of heat transfer points.

Step 1	32, 34, 86, 92.
Step 2	41, 43, 57Y.
Step 3	57X, 62, 63X, 63Y.
Step 4	71, 75.

Table 4 – Range of variation in temperature.

Temperature	Range (°C)
Room temperature	25–27
Hydrolysis	425–450
Oxygen decomposition	500–550

Genetic algorithm

The genetic algorithm (GA) is a member of evolutionary algorithms (EA), it mimics the genetics and process of natural selection, such as inheritance, mutation, selection, and crossover, to generate solutions to optimization and searching problems. A GA allows a population composed of many individuals to evolve under specified selection rules [24], by doing so, some inherent features which maximizes the "fitness" (i.e., minimizes the cost function) are kept to generate optimum solutions.

Like any other optimization algorithm, GA starts by defining variables and cost of objective optimization problems, and ends by testing for convergence, however, some particular steps in between make it different from others. Fig. 4 gives the flowchart of GA, some of the steps are explained briefly afterwards.

The ranges of the variables: since the 4-step whole Cu–Cl cycle is an endothermic process, for most of the input and output temperatures at each heat transfer point, the required heat decreases with the temperature rising up, so only the lower boundary of each variable need to be decided to find out whether the heat provided can satisfy the requirement or not. However, as can be seen from Table 1, the highest temperature the system requires is 550 °C which is the oxygen decomposition temperature, and at heat transfer point 71 and 75, when the oxygen decomposition temperature is getting closer to 550 °C, though the heat requirement for heat transfer point 71 is increasing, the amount of heat point 75 releases will drop more drastically. Therefore, for oxygen

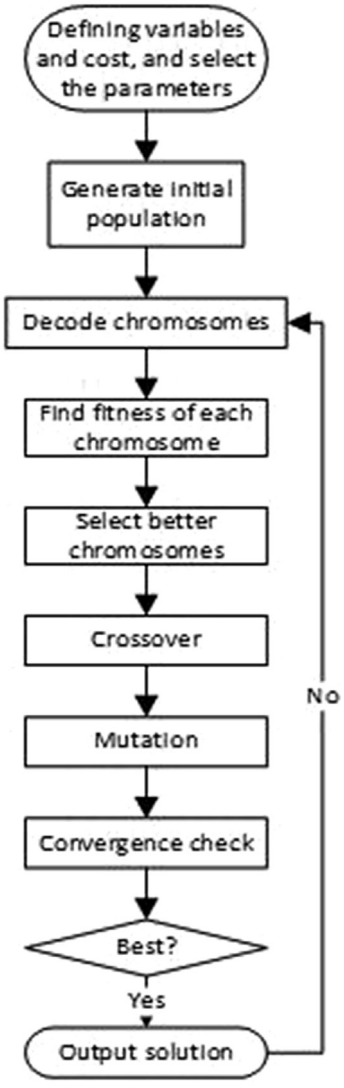

Fig. 4 – Flowchart of genetic algorithm.

decomposition temperature, the optimal upper boundary need to be found to make sure more heat is released from point 75 than it required by point 71. In conclusion, the variables to be optimized are defined and shown in Table 5. In the table, T_1 is the varying room temperature, T_2 and T_3 stands for hydrolysis temperature and oxygen decomposition temperature respectively.

Selection: This step occurs in each iteration of the algorithm. It aims at keeping the individuals with high fitness and discarding the ones with lower fitness. The selection rate which is arbitrarily defined in this step decides the proportion of chromosomes that will survive. Many methods can be used to perform the selection, like rank selection, tournament selection, roulette wheel, Elitism Selection and Stochastic Universal Sampling. In this paper, roulette wheel selection is chosen to be used.

Crossover: This step is to interchange genes in chromosomes to create offspring and increase diversity of the population. Usually, a crossover point is randomly selected in two chromosomes, offspring1 will get the genes before the crossover point of parent1 and the genes after the crossover point of parent2, in a like manner, offspring2 will get the genes before the crossover point of parent2 and the genes after the crossover point of parent1. In this way, the population size is raising, also, the offspring keep the good genes which maximize the fitness.

Mutation: This step will change one or more randomly selected genes in chromosomes in order to introduce traits not in the original population and keeps the GA from converging too fast before sampling the entire cost surface [24].

MCS-based performance analysis

For a newly built system, performance analysis is of paramount importance, since it is able to reflect the actual performance of the whole nuclear-based hydrogen production [14,25,26]. Moreover, after global searching, GA will output a result which gives the optimal ranges of the varying temperatures. However, there should be a way to evaluate the optimality of the result, in other words, to decide whether a range is optimal or good enough that the system will operate safely no matter how the temperatures change in that range. In this case, performance analysis is an appropriate way to assess the feasibility and stability of the solution, and the pass rate can also be used as a criterion for GA. So when a result pass the criterion, it means that faults are less possible to take place in the system when the temperatures change in the range. In this paper, Monte-Carlo Simulation (MSC) based performance analysis is applied to evaluate the reliability of the GA simulation solutions. Fig. 5 gives the flowchart of MSC-based performance analysis.

Table 5 – The range of each variable to be optimized.

Variables	Ranges (°C)
Room temperature	T_1–27
Hydrolysis temperature	T_2–450
Oxygen decomposition temperature	500–T_3

The main idea of MSC-based performance analysis is to solve an engineer or mathematical problem by building a probabilistic model. The process is described briefly as following:

1. Determine the evaluation criteria which in this case is the required heat: 543.8 kJ.
2. Decide the probability distribution the input variables follow. For some particular cases, if it cannot be decided due to sparse data or other reason, one can assume the variables following a uniform distribution.
3. Randomly sample data based on the particular probability distribution.
4. Calculate the target value of the overall heat transfer function with data generated from step 3.
5. Compare the calculation result with the heat requirement and note down the number of passed samples.
6. Repeat step 3 to step 5 until a predetermined iteration time is reached.
7. Output the simulation results and calculate the pass rate.

GA-based MCS method

In the light of the illustrations outlined above, it is reasonable to develop a method as shown in the flowchart in Fig. 6.

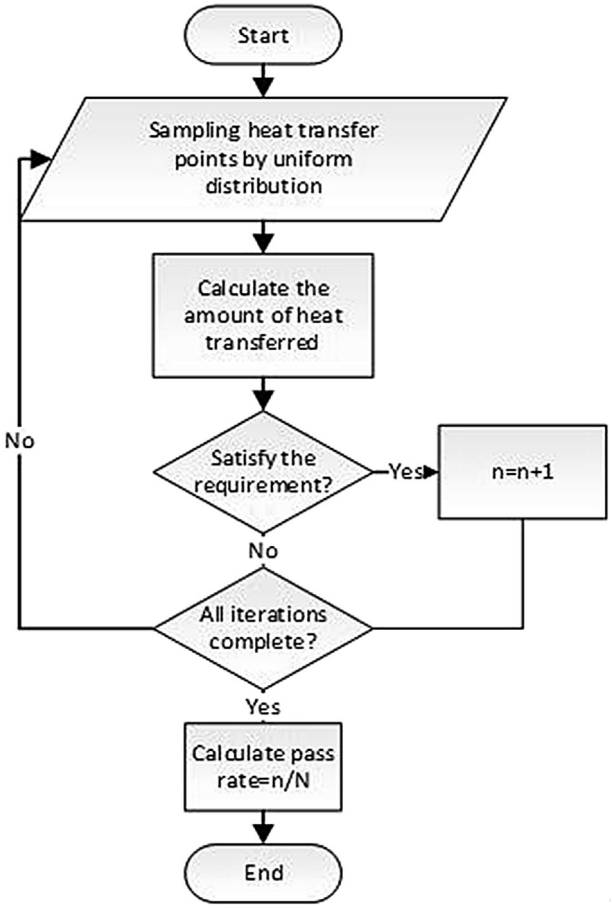

Fig. 5 – Flowchart of MSC-based performance analysis.

As can be seen from Fig. 6, the flowchart in the red block is MCS-based performance analysis which is used to evaluate the reliability of the solutions generated by GA operator. The fitness function of GA is defined based on the result of MCS-based performance analysis. The process of defining the transfer function of MCS method and the fitness function of GA will be shown in next section.

Transfer function and fitness function

As mentioned above, the most important step of GA-based MCS method is to identify the fitness function, in other words, to identify the objective to be optimized. The object is to modify the output in some desirable fashion by finding the appropriate values for the input variables [24].

In order to define the fitness function of GA, it is important to calculate the heat transfer function at each heat transfer point first.

The standard heat transfer function is shown as follow:

$$Q = cp \cdot m \cdot \Delta T \tag{4}$$

In the function, cp is the heat capacity of chemicals involved, m stands for the mass of those chemicals, and ΔT is the temperature difference between input and output. Since only the heat capacity of CuCl is seen as a variable changing with the temperature as mentioned previously, heat capacity of all other chemicals are considered to be constants during the process. Moreover, the mass of each chemical is fixed, so the only changing parameter in heat transfer function is ΔT. Therefore, the productions of cp and m can be considered as constant which can be obtained from Table 1. For example, for heat transfer point 63Y, the heat consumed is 55.382 kJ, ΔT is 398 °C, so the production of cp and m should be 55.382 kJ/398 °C, which is 0.1392 kJ/°C. Therefore, the heat transfer function at point 63Y is:

$$Q_{63Y} = 0.1392 \cdot \Delta T_{63Y} \tag{5}$$

Furthermore, the only heat transfer point associated with CuCl is point 75. CuCl generated from previous steps will be cooled down at this point. At heat transfer point 75, only part of the energy is consumed or recovered by CuCl generated from step 1 and step 4, the rest is required by other chemicals whose heat capacity can be seen as constants. According to the simulation result, CuCl recycled from step 1 is 450 °C, and from step 4 is 550 °C. Therefore, the heat recovered by cooling down CuCl can be calculated with Eqs. (1)–(3) and shown as follow:

$$\begin{aligned} Q_{CuCl} = m \cdot \left(\int_{685}^{298.15} cp_1 dT + \int_{696}^{685} cp_2 dT + \int_{823.15}^{696} cp_3 dT + \int_{685}^{298.15} cp_1 dT \right. \\ \left. + \int_{696}^{685} cp_2 dT + \int_{723.15}^{696} cp_3 dT \right) \\ = -27.055kJ \end{aligned} \tag{6}$$

Since CuCl is recycled from two steps, m is 2 mol. Therefore, heat transfer function for the rest at point 75 is:

$$Q_{rest} = \frac{-27.189 - (-27.055)}{25 - 550} \cdot \Delta T = 6.476 \times 10^{-5} \cdot \Delta T_{75} \tag{7}$$

In conclusion, with variations in the temperatures, the heat transfer function at heat transfer point 75 is:

$$Q_{75} = Q_{CuCl} + Q_{rest} \tag{8}$$

In the same manner, the heat transfer functions at other heat transfer points are shown in Table 6:

As can be seen, at some particular heat transfer points, there is no variation in the input or output temperatures, therefore, the heat transfer functions are shown as constants in the table.

The heat transfer function for the overall process can be calculated by summing all heat transfer functions up with the following equation:

$$Q_{total} = \sum Q = 1.406 \cdot T_1 + 1.346 \cdot T_2 + 0.0447 \cdot T_3 + Q_{75} - 61.533 \tag{9}$$

For Q_{total}, with the temperatures varying, the value of it should be lower than the heat provided from the nuclear power plant which is 543.8 kJ according to the simulation result. Therefore, for performance analysis, it is reasonable to define the objective function as follow:

$$Q_{MCS} = 543.8 - Q_{total} \tag{10}$$

With random values for each variable generated in a certain range, whenever the result of Eq. (10) passes 0, the number of passed sample will be added by 1. However, the pass rate of performance analysis should not be too high, otherwise the GA operator will tend to generate higher values for the variables in a certain range to achieve the pass rate in each iteration of MCS-based performance analysis, which will no doubt affect the accuracy of the optimal ranges. Therefore, the required pass rate for performance analysis should be defined with paramount concern. A pass rate of 0.985 is an acceptable number, since it can not only guarantee a good performance of the system, but also avoid an immature convergence. Therefore, the fitness function for GA should be define as follow:

$$fitness = |pass\ rate - 0.985| \tag{11}$$

The lower the value of the fitness function is, the closer to 0.985 the pass rate is, the more desirable the result is. Therefore, the GA operator will search for values for the three variables to make the value of fitness function as low as possible.

Results and analysis

Results

The parameters of GA-based MCS method are chosen as shown in Table 7.

The model of GA-based MCS method is built based on the parameters in Table 7. The best individual of each variable in every generation is acquired and shown in Figs. 7–9.

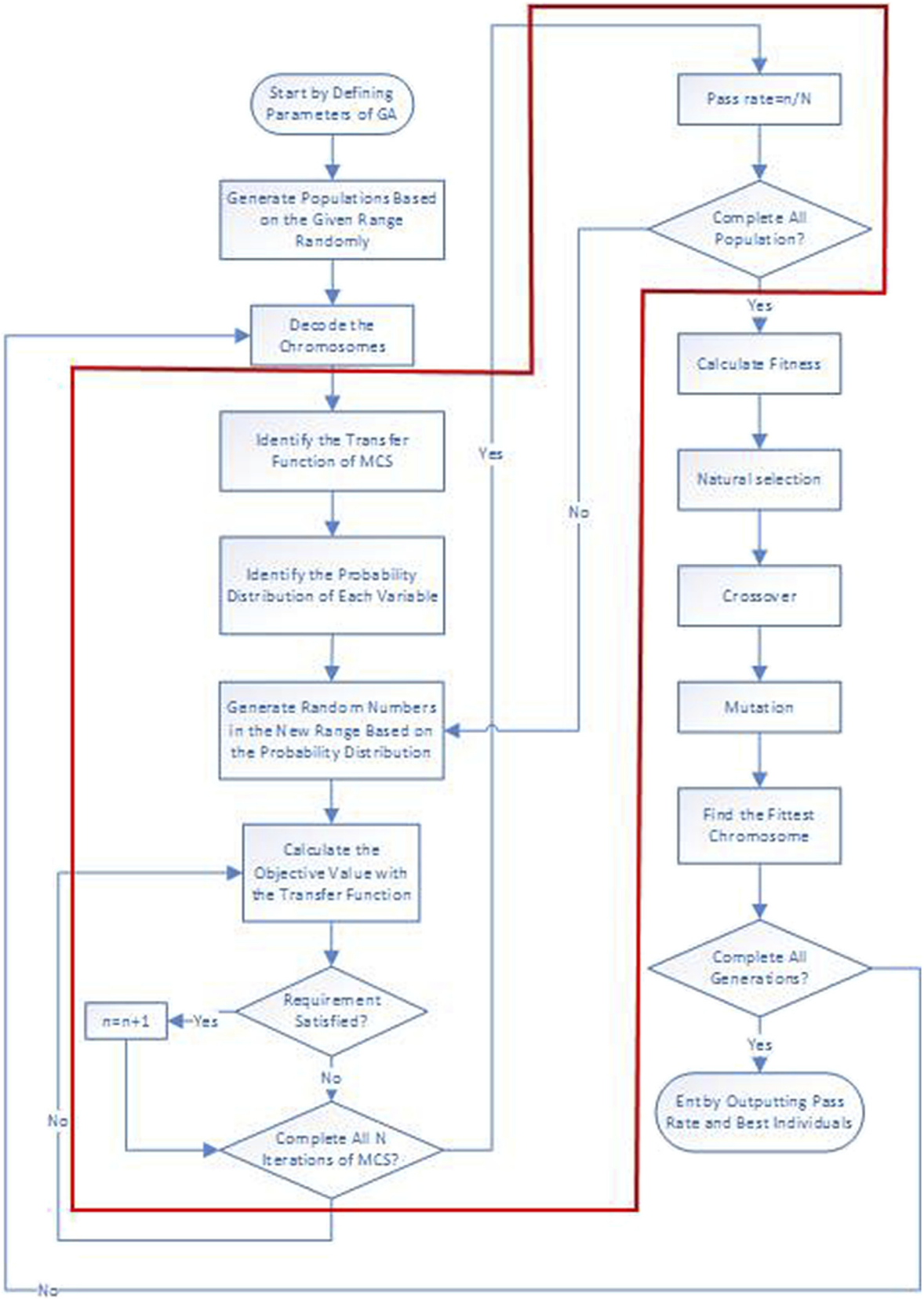

Fig. 6 – Flowchart of GA-based Monte Carlo Simulation method.

As can be seen from the figures above, for the room temperature, the best individual of the first few generations stays at 25.5714 °C, at the 5th, 6th and 7th generation, it jumps to 25.8571 °C, then quickly drops to 25.5714 °C again, and rises to and stays at 25.8571 °C. This means that firstly, the process of crossover and mutation are able to introduce diversity to the

Table 6 – Heat transfer function at each heat transfer point.

Heat transfer points	Heat transfer functions
32	$0.999 \cdot \Delta T_{32} = 0.999 \cdot (100 - T_1)$
34	244.092 kJ
41	−231.860 kJ
43	$0.354 \cdot \Delta T_{43} = 0.354 \cdot (T_1 - 105)$
57X	−107.365 kJ
57Y	320.923 kJ
62	−15.526 kJ
63X	$1.539 \cdot \Delta T_{63X} = 1.539 \cdot (T_1 - 90)$
63Y	$1.391 \cdot \Delta T_{63Y} = 1.391 \cdot (T_2 - T_1)$
71	$0.0447 \cdot \Delta T_{71} = 0.0447 \cdot (T_3 - T_2)$
75	$Q_{75} = Q_{CuCl} + Q_{rest}$
86	0.351 kJ
92	$1.904 \cdot \Delta T_{92} = 1.904 \cdot (T_1 - 117)$
Auxiliary	26.4 kJ

population, though the new chromosome is not fit enough sometimes; secondly, even though the results start from 25.5714 °C and drop to it later, 25.8571 °C survives at last, which means comparing to 25.8571 °C, 25.5714 °C is less fitter; lastly, the figure only shows the best individual of each generation, crossover and mutation may take place many times, however, only 25.8571 °C survives at last, which means the result is trustable enough.

For the same reason, the result of T_2 as shown in Fig. 8 is also credible, plus, the results of T_2 also prove that the population size is sufficiently large, which makes the operator be able to find the optimal solution for T_2 in the first generation.

For the oxygen decomposition temperature T_3, the result in Fig. 9 shows more fluctuation than T_1 and T_2, since for one thing, the length of chromosomes of T_3 is longer than that of T_1 and T_2, and for another thing, the span of the range of oxygen decomposition temperature is much larger, which makes the searching space of T_3 much larger. However, the result of T_3 shows high stability in the middle few generations, though a little fluctuation after, it becomes stable in the last generation, which also prove the result is trustable.

After simulation, the fittest solution for each variable is listed in Table 8. The optimal ranges for all temperatures can be decided with the results in Table 8 and are shown in Table 9.

Table 9 indicates that whenever the room temperature drops below 25.8571 °C, there may exist a potential problem in the system that the heat provided from the NPP may not satisfy the heat requirement of the hydrogen production system, so the operators should pay attention to this problem and take actions, such as reduce the amount of chemicals of the reactions or ask for more heat, to avoid negative effects. In

Table 7 – Parameters of GA-based MCS method.

Parameters	T_1	T_2	T_3
Number of iteration of GA	100		
Number of iteration of MCS	800		
Population size	50		
Chromosome length	3	4	5
Crossover rate	0.5	0.5	0.6
Mutation rate	0.01	0.04	0.04

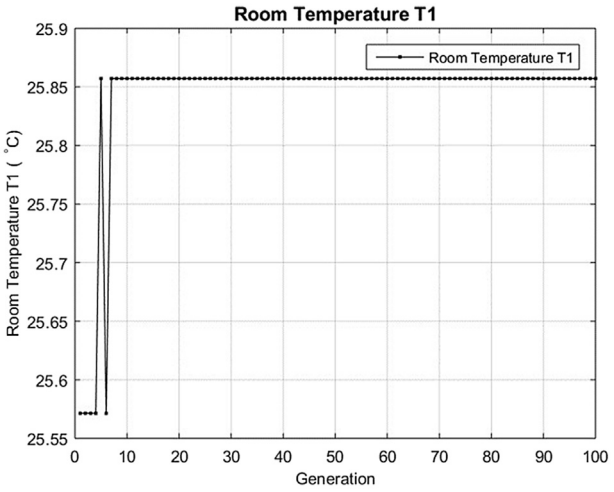

Fig. 7 – Best individuals of T_1 in each generation.

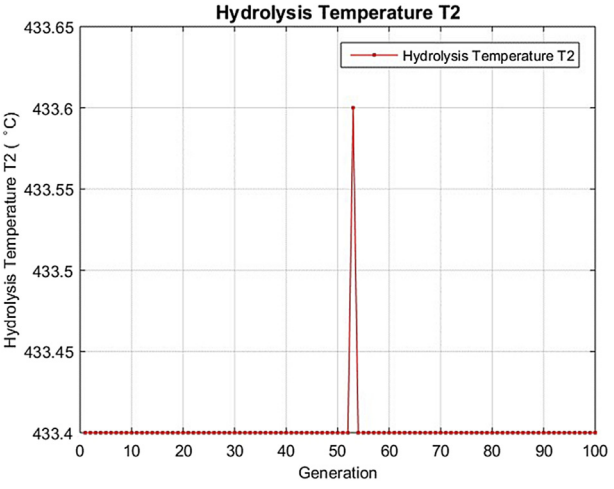

Fig. 8 – Best individuals of T_2 in each generation.

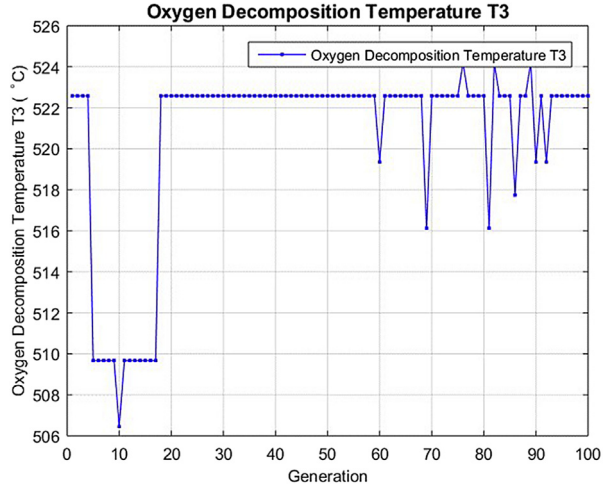

Fig. 9 – Best individuals of T_3 in each generation.

the same manner, whenever the hydrolysis temperature drops below 433.4 °C or the oxygen decomposition temperature rises above 522.875 °C, there should be an alarm to inform the operators to deal with the problems.

Fig. 10 shows the pass rate of performance analysis in each generation, as can be seen from the figure, the pass rate of performance analysis sometimes fluctuates with the variables. The appropriate pass rate setting makes the heat provided from the NPP sufficient for the system in almost all cases, and makes sure the GA operator not tend to generate low values for the temperatures to achieve high pass rate.

Confidence interval estimation

Variation in results is an important factor when evaluate the reliability of the results. GA-based MCS method is not an exception. The confidence interval of results will show the interval of true value of the final results [14]. If the simulation results have relatively small variations, the range of the confidence interval will also be small. Therefore, it can evaluate the accuracy of the results based on simulation.

In statistics, confidence interval is the estimates of population of a probability sample [27]. Confidence interval indicates the probability of the true value locates in a certain interval. For instance, if the 95% confidence interval of parameter A is [62, 63], it means that the true value of parameter A has a probability of 95% to fall in the interval [62, 63] [28].

If the size of the sample is over 30, the confidence interval of the results can be defined by the confidence interval estimates of population parameters [29,30]. Therefore, the GA-based MCS method for optimal range identification is executed for 30 times. The results for each variable are shown in Table 10.

The means and standard deviations of all three temperatures are calculated and shown in Table 11.

The mean and standard deviation are denoted by μ and σ respectively for convenience. 95% confidence interval is widely applied in most statistical problems, it can be calculated with the following equation:

$$\text{confidence interval} = \mu \pm Z_{\frac{\alpha}{2}} \cdot \frac{\sigma}{n} \tag{12}$$

In Eq. (12), n is the number of the samples, μ is the mean of the samples, σ stands for the standard deviation, $Z_{\frac{\alpha}{2}}$ is the value from the standard normal distribution for the selected confidence level (e.g., for a 95% confidence level, $Z_{\frac{\alpha}{2}} = 1.96$) [31]. The 95% confidence interval of each variable is calculated and shown in Table 12.

As can be seen from Table 12, the 95% confidence interval of T_1 is [25.705, 25.809], which means the probability of T_1 locating in [25.705, 25.809] is 95%. Similarly, the probability of T_2 locating in [433.595, 434.245] is 95%, the probability of T_3 locating in [521.645, 528.415] is 95%. The span of each interval is 0.104, 0.65 and 6.77 respectively, which are only 0.402%, 0.145% and 1.29% of the optimal solution, which means the results are stable and trustable.

Additionally, the resolution for platinum RTDs are ±0.5 °C, ±2.5 °C and ±2.8 °C respectively according to IEC-751. In order to detect all potential faults, the optimal ranges for three temperatures can be further improved with the help of confidence interval as follows:

As can be seen from Table 13, with the help of confidence interval, the optimal ranges for temperatures are improved. Although the span of the improved ranges are smaller comparing to the ones shown in Table 9, especially for T_1, they can make sure all potential faults be detected.

Table 8 – The fittest solution for each variable.

Temperature	Best solution
T_1	25.8571
T_2	433.4
T_3	522.875

Table 9 – The optimal range for each temperature.

Temperature	Optima range (°C)
Room temperature	[25.8571, 27]
Hydrolysis temperature	[433.4, 450]
Oxygen decomposition temperature	[500, 522.875]

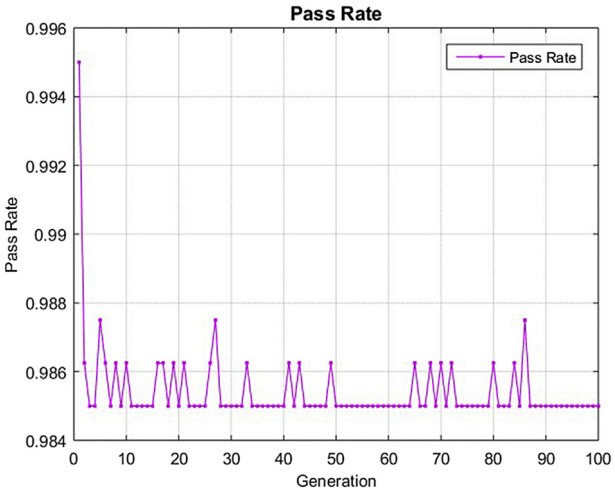

Fig. 10 – Pass rate of performance analysis in each generation.

Conclusions

This paper aims at identifying the optimal ranges for three temperatures in the heat transfer process of a nuclear hydrogen production system based on a 4-step Cu–Cl cycle. Genetic-algorithm-based Monte Carlo simulation method is developed in the paper to deal with the target problem. The model of GA-based MCS method is first established and applied to a power system, the process of modeling is presented and illustrated in detail. Afterwards, the method is applied to the heat transfer process of the objective system, the optimal ranges of three varying temperatures in the process, namely room temperature, hydrolysis temperature and oxygen decomposition temperature, are found and proved to be reliable.

Table 10 – Results of 30 experiments.

Experiment	T_1 (°C)	T_2 (°C)	T_3 (°C)	Experiment	T_1 (°C)	T_2 (°C)	T_3 (°C)
1	25.8571	433.400	522.875	16	25.8571	433.400	522.875
2	25.8571	435.000	536.568	17	25.9325	433.400	509.677
3	25.8571	433.400	522.875	18	25.8571	435.000	536.568
4	25.5714	433.400	522.875	19	25.8571	433.400	522.875
5	25.5714	436.712	540.223	20	25.8571	433.400	522.875
6	25.8571	433.400	522.875	21	25.5714	433.400	508.065
7	25.9325	433.400	536.568	22	25.8571	435.000	522.875
8	25.8571	433.400	522.875	23	25.5714	433.400	540.223
9	25.8571	433.400	508.065	24	25.8571	435.000	536.568
10	25.5714	433.400	522.875	25	25.5714	432.771	522.875
11	25.5714	435.000	522.875	26	25.8571	435.000	522.875
12	25.8571	433.400	541.936	27	25.8571	433.400	508.065
13	25.5714	435.000	522.875	28	25.5714	433.400	522.875
14	25.8571	433.400	522.875	29	25.8571	433.400	522.875
15	25.5714	435.000	536.568	30	25.5714	433.400	522.875

Table 11 – Mean and standard deviation of each variable.

Temperature	Mean	Standard deviation
T_1	25.757	0.145
T_2	433.92	0.907
T_3	525.03	9.46

Table 12 – 95% confidence interval of each variable.

Temperature	95% confidence interval
T_1	[25.705, 25.809]
T_2	[433.595, 434.245]
T_3	[521.645, 528.415]

Table 13 – Improved optimal range for each temperature.

Temperature	Optimal range (°C)
Room temperature	[25.809 + 0.5, 27] = [26.309, 27]
Hydrolysis temperature	[434.245 + 2.5, 450] = [436.745, 450]
Oxygen decomposition temperature	[500, 521.645−2.8] = [500, 518.845]

Acknowledgment

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Nomenclature

aq	aqueous
c_p	heat capacity, J/mol °C
g	gas
GA	genetic algorithm
l	liquid
m	mass of the chemicals, mol
MCS	Monte-Carlo simulation
Q	heat, kJ
s	solid
T	temperature, °C

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