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Abstract: In order to explore the hydrogen source term characteristics under severe accidents of marine pressurized water reactors (PWR) and effectively assess the hydrogen risk, the best estimation program SCDAP/RELAP5/MOD3.2 is used to establish the marine reactor severe accident analysis model. Based on the Latin Hypercube sampling (LHS) method and the Wilks sampling theory, a set of methods for the uncertainty analysis of severe accidents is developed. This method can be applied to the uncertainty and sensitivity analysis of different target parameters. The phenomenon identification and ranking table (PIRT) under the severe accident induced by the break are established, and 14 uncertain parameters are selected as input variables. The established PIRT fills the gap in the uncertainty and sensitivity analysis of severe accidents of marine reactors and provides a reference for subsequent research. The quantitative uncertainty analysis of the calculation results is carried out, and the uncertainty range of hydrogen production is defined. The Spearman correlation coefficient is used to evaluate the sensitivity of input parameters, and the sensitivity of each parameter to hydrogen production is obtained. The results show that under the severe accident caused by the medium equivalent diameter break, the uncertainty range of hydrogen production in the zirconium-water reaction in the pressure vessel is 20.14 kg~22.19 kg with 95% confidence, and the fuel cladding thickness has a significant positive correlation on the hydrogen production.

Keywords: marine PWR; severe accident; hydrogen source term; uncertainty analysis; sensitivity analysis

1. Introduction

The hydrogen source item under the severe accident of nuclear reactor is one of the hot issues of international concern. The response process of the Three Mile Island (TMI) nuclear accident [1,2] and the Fukushima nuclear accident [3–5] shows that the production of hydrogen and its behavioral characteristics under severe accident conditions of light water reactor (LWR) have an important impact on the accident process. The factors affecting the oxidation of hydrogen production at the reactor core are very complex, and there is great uncertainty in the hydrogen source term. The uncertainty analysis of the hydrogen source term is carried out to facilitate a more accurate assessment of hydrogen risk and accident consequences, and it is of great significance for the mitigation of severe accidents [6,7].

At present, a large number of uncertainty analyses of typical phenomena under severe accidents have been carried out at home and abroad. Tsinghua University in Taiwan took the boiling water reactor (BWR) of Longmen nuclear power plant as the research object and adopted the MAAP program to carry out uncertainty analysis of the hydrogen source term in the pressure vessel under severe accidents according to the model parameters, such as the porosity of the debris bed [8]. Yuan et al. selected severe accidents caused by station blackout (SBO) in a 600 MW nuclear power plant and calculated the uncertainty envelope of hydrogen production in the pressure vessel by using the MELCOR program, and identified the input parameters with greater sensitivity [9]. Gharari et al. selected the WWER1000/V466 four-loop pressurized water reactor as the research object and used the MELCOR program to study the uncertainty of hydrogen generation during severe



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Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). accidents [10–12]. Darnowski et al. used MELCOR to perform uncertainty and sensitivity analyses for a Gen-III PWR and Phebus FPT-1 to study in-vessel stage hydrogen production in a severe accident in a light water reactor [13]. Mazgaj et al. used MELCOR to analyze the uncertainty and sensitivity of the hydrogen production process for Phebus FPT-1 [14]. Itoh H et al. adopted the severe accident analysis program MELCOR and took the accident of Unit 2 of the Fukushima Nuclear Power Plant as an example. Under the assumption of drywell failure, the uncertainty distribution of the total mass output of hydrogen production in the reactor pressure vessel was obtained by uncertainty analysis [15]. It can be seen from the above research results that for reactors of different structures, there may be differences in the simulation of hydrogen behavior under severe accidents by different analysis programs. Compared with the existing methods, the main highlights of the proposed research scheme are outlined as follows:

- (1) In this paper, the mechanical rational program SCDAP/RELAP5/MOD3.2 is selected as the tool for severe accident analysis. Compared with MAAP and MELCOR, the real physical model of the SCDAP/RELAP5/MOD3.2 program can more accurately describe the physical phenomena in the process of severe accidents [16].
- (2) A severe accident analysis model for marine PWR is established in this paper. Additionally, based on the LHS method and Wilks sampling theory, a set of uncertainty analysis method flow for marine PWR severe accidents is developed. This method can be applied to the uncertainty and sensitivity analysis of different target parameters.
- (3) In this paper, the PIRT for severe marine reactor accidents is established, and the uncertain parameters affecting the target parameters are selected as input variables. The established PIRT fills the gap in the uncertainty and sensitivity analysis of severe accidents of marine reactors and provides a reference for subsequent research.

Therefore, this paper focuses on the severe accidents caused by breaks in a marine pressurized water reactor. Firstly, a severe accident analysis model is established, and the established model is verified according to the steady-state and transient-state results, and on that basis, the phenomenon identification of influencing factors of hydrogen source term is carried out, the ranking table is established, and the range and probability distribution of input parameters are determined. After that, the best estimation program, SCDAP/RELAP5//MOD3.2, is used to carry out batch sampling analysis, and the set of output results is obtained. Finally, the uncertainty analysis of hydrogen source terms under severe accidents is carried out, and the Spearman correlation coefficient is used to evaluate the sensitivity of uncertain input parameters to the hydrogen production in the reactor.

2. Model Establishment and Verification

The purpose of volume partition is to discretize the described system in space coordinates so that the program can simulate the response of a complex system. The more volumes are divided, the more detailed the program describes the internal characteristics of the system, but the more computing resources are required. Therefore, the calculation accuracy and calculation time must be considered comprehensively in practical engineering applications [17].

The marine nuclear power plant is mainly composed of a nuclear reactor, primary system, secondary system, propulsion shafting and related instrumentation, control system, etc. Compared with the PWR of the nuclear power plant, it is smaller in size, lower in power and compact in space arrangement. According to the design and operation parameters of a certain type of marine pressurized water reactor, the system analysis model was established by using the severe accident analysis program SCDAP/RELAP5//MOD3.2 [18]. The schematic diagram of the model is shown in Figures 1 and 2. Figure 1 shows the node diagram of the reactor coolant system. The system has two parallel loops, each of which includes a steam generator (207/407). A pressurizer (600) is connected in a loop to adjust the pressure change in the system. The main pipe of the loop is connected with the inlet and outlet of the pressure vessel to form a closed-loop system; Figure 2 shows the reactor core volume diagram inside the pressure vessel. The main factor affecting the core damage

process during serious accidents is reactor power. In this paper, fuel assemblies were divided into four zones according to the core power factor, and each zone has the same equivalent power factor. Then, the steady-state calculation of 100% rated power operating condition was carried out. The comparison between calculation results and design values is shown in Table 1. It can be seen that the relative errors between the steady-state calculation results and the design values of each macro characteristic parameter meet the needs of engineering simulation, and the correctness of the model is preliminarily verified.



Figure 1. Analysis model of coolant system.



Figure 2. Analysis model of reactor core.

When the hot leg of the primary coolant system is broken, the coolant flows through the core and loses from the break, and the heat can be taken away from the core at the same time. When the cold leg of the primary coolant system is broken, a large amount of coolant cannot take away the core heat when it is lost through the break. At this time, the continuous accumulation of core heat may cause core damage. Therefore, under the same break size, LOCA occurs in the cold leg will lead to more serious consequences.

Parameter Description	Unit	Nominal Value	Relative Error
Reactor power	MW	1.0	0%
Core water level	m	1.0	0%
Regulator pressure	MPa	1.0	0.07%
SG secondary pressure	MPa	1.0	0.42%
SG secondary steam flow	kg/s	1.0	0.88%
Core inlet flow	kg/s	1.0	0.51%
Core outlet flow	kg/s	1.0	0.49%
Core inlet temperature	K	1.0	0.23%
Core outlet temperature	K	1.0	0.11%

Table 1. Comparison between calculated value and design value.

In order to analyze the uncertainty of the transient state of subsequent accidents, the break model was added to the severe accident analysis model established in this paper. On the basis of steady-state verification, transient simulation of LOCA under 100% rated power operation was carried out using the established model, and the variation curves of some important parameters in the calculation results were compared with the safety analysis report. In this paper, it was assumed that a break with an equivalent diameter of 38 mm occurs in the cold leg of the primary coolant system, and the transient running time was set to 3000 s. By analyzing the calculation results, it can be found that the variation curve of important parameters over time is basically consistent with the safety analysis report. The availability of the break model and its ability to simulate the LOCA response process was verified.

Figure 3 shows the variation curve of the pressurizer pressure over time, Figure 4 shows the variation curve of the core water level over time and Figure 5 shows the variation curve of the break coolant flow over time. After LOCA occurs, coolant spews out through the break. When the water level of the pressurizer is reduced to the setting value, the high-pressure safety injection system is automatically put into operation. There is a brief increase in pressure on the pressurizer (as shown in Figure 3). The primary system pressure continues to decrease as the safety injection flow is less than the coolant flow through the break. When the pressure drops to the low-pressure injection safety system input setting value, the system is automatically put into operation to ensure effective core cooling (As shown in Figure 4).



Figure 3. The variation curve of the pressurizer pressure over time.



Figure 4. The variation curve of the core water level over time.



Figure 5. The variation curve of the break coolant flow over time.

3. Process Analysis of Severe Accident Induced by LOCA

Typical marine reactor severe accident sequence mainly includes the whole ship power failure and LOCA superimposed safety injection system failure, etc. In the event of a whole ship power failure, the safety valve will be triggered to open, and the coolant will be discharged into the sea through the safety valve of the pressurizer. The hydrogen produced during the accident is likely to be released directly into the environment, mainly through the safety valve, so there is no risk to the reactor cabin. For this reason, this paper chose the severe accident sequence caused by LOCA as the research focus and selected a medium-size break with an equivalent diameter of 38 mm according to the safety analysis report to carry out the research.

After LOCA occurs in the marine reactor, a large amount of high-temperature and high-pressure coolant is released into the reactor cabin through the break. When the water level of the pressurizer is reduced to the setting value, the high-pressure safety injection system is automatically put into operation. If the high-pressure safety injection coolant flow is less than the break coolant flow, the primary system pressure will continue to decrease. When the pressure drops to the low-pressure injection safety system input setting value, the system is automatically put into operation to ensure effective core cooling. After the occurrence of LOCA, the working environment of the reactor cabin is very harsh, and there is great uncertainty about whether the safety injection system can operate effectively. If the safety injection system is not operational, the continued loss of coolant will result in an exposed core and rapidly deteriorating heat transfer conditions in the core. The fuel cladding temperature increases continuously under the heating of decay heat.

When the fuel cladding temperature reaches 1000 K, zirconium in the reactor begins to oxidize with high-temperature water vapor [19]. The oxidation reaction produces hydrogen and releases a lot of oxidation heat. The core temperature rises further under the heating of decay heat and oxidation heat. With the development of the core melting process, the fuel cladding will swell and break. The resulting debris will migrate, which will block part of the coolant flow path, and the core damage process is aggravated due to insufficient core cooling. Hydrogen production is closely related to the quality of zirconium, the quality of water vapor, the temperature of fuel cladding and the damage degree of the core, so the influencing factors are very complex. Therefore, it is necessary to analyze the uncertainty and sensitivity of hydrogen production.

4. Uncertainty Analysis Methods

The best estimation plus uncertainty (BEPU) analysis method refers to the method that adopts the best estimation program to accurately simulate the real situation of the reactor through realistic physical models and evaluate the confidence interval of the analysis results through uncertainty analysis. Compared with conservative evaluation methods, the BEPU method can release more safety margins on the premise of ensuring safety [20,21]. During the transient response to the accident, the source of uncertainty mainly includes the uncertainty of initial and boundary conditions, the uncertainty of the accident phenomenon, the uncertainty of the influence of the operator's behavior on the accident process, and the uncertainty caused by cognitive limitations on the physical parameters of the program model due to incomplete understanding of the severe accident phenomenon.

The input uncertainty propagation method [22] refers to the process of input uncertainty propagation through the best estimation program, and the input uncertainty is generally represented as the uncertainty range and probability density distribution of the input parameters. In this method, the input parameters are sampled based on the appropriate sampling method, and then the transient process of the accident is simulated by the estimation program. Finally, the uncertainty and sensitivity of the output results are analyzed. Figure 6 shows the flow chart of the uncertainty analysis method.



Figure 6. Flow chart of uncertainty analysis method.

4.1. Parameter Sampling Method

The sampling methods commonly used in uncertainty analysis include the simple random sampling (SRS) method and the LHS method [23]. The LHS method divides the range of input parameters into multiple equal probability and non-overlapping intervals, and samples are selected from each interval, respectively, and then uncertainty transfer calculation is carried out after random combination. Compared with the SRS method, the samples selected in the LHS method are more evenly distributed and can better reflect the distribution characteristics of random variables. Therefore, the LHS method is more efficient in uncertainty calculation, and this paper chooses the LHS method for further research.

Currently, the common methods used for quantifying uncertainty include a parametric statistical method, an Owen factor method, a non-parametric statistical method, an alternative model method, a sensitivity analysis method, etc. [24]. According to the characteristics of the studied problem, this paper selects the non-parametric statistical method to carry out the analysis. The non-parametric statistical method does not depend on the distribution type of the continuous distribution population, and the number of sampling is not directly related to the number of input parameters but only related to the allowable limit and confidence level of the output results. In order to effectively reduce the calculation cost for the unilateral tolerance limit of a single output parameter, the sample size can be calculated based on the Wilks [25] formula to solve the required number of samples at a certain confidence level:

$$\beta = 1 - \gamma^N \tag{1}$$

In the above equation, β represents the confidence level, γ represents the probability share of the allowable limit, and *N* represents the number of calculations. When $\beta = \gamma = 0.95$, it was established that *N* = 59. It means that at least 59 sample analysis calculations need to be successfully completed in order to meet the "95/95 criteria" for safety analysis.

4.2. PIRT Establishment and Parameter Selection

There are many input parameters involved in the dynamic response process of severe accidents caused by marine PWR break, which can be macroscopically divided into initial state parameters, accident characteristic parameters and response intervention parameters. Due to various limitations, it is difficult to consider the uncertainty of all parameters in the actual analysis process, so it is necessary to screen out the parameters that have a greater impact on the target parameters based on certain methods. The commonly used method is to establish the phenomenon identification and ranking table according to the safety analysis report of marine PWR, relevant research results and literature, expert research judgment or reference to the engineering experience of similar reactors. The main phenomenon characteristics of PIRT in severe accidents caused by breaks include the characteristics of the initial accident, the characteristics of core heat source and heat transfer behavior, the characteristics of coolant loss, the geometric structure characteristics of the fuel rod, the characteristics of debris after core melting, the characteristics of safety injection, etc. By analyzing the above phenomenon characteristics one by one, this paper identifies 14 uncertain input parameters for the research object. The description of specific parameters is shown in Figure 7.

4.3. Input Parameter Range and Distribution

According to the analysis in Section 4.2 and combined with the analysis and the engineering judgment of the accident process in the pressure vessel of severe accidents, this paper selects 14 uncertain parameters that have an important influence on the hydrogen source term during the coolant loss process, the core melting and relocation process, and the debris bed formation process. After determining the range of input parameters, probability density distribution and other statistical characteristics, uncertainty analysis is carried out. The results of the normalization of some parameters are shown in Table 2.



Figure 7. The description of uncertain input parameters.

Table 2. Distribution and range of uncertain input parameters.
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Serial Number	Parameter Name	Nominal Value	Type of Distribution	Value Range
1	Break size (m ²)	1.0	Uniform	(0.9, 1.1)
2	Break resistance coefficient	1.0	Uniform	(0.9, 1.1)
3	Reactor power (MW)	1.0	Uniform	(0.97, 1.03)
4	Power peak factor	1.0	Uniform	(0.97, 1.03)
5	Core resistance coefficient	1.0	Uniform	(0.9, 1.1)
6	Safe injection water temperature multiplier	1.0	Uniform	(0.9, 1.1)
7	Safe injection water flow multiplier	1.0	Normal	$\sigma = 0.03$
8	Fuel rod gas gap size (mm)	0.075	Normal	$\sigma = 0.0025$
9	Fuel rod cladding thickness (mm)	0.5	Normal	$\sigma = 0.017$
10	Fuel rod internal pressure coefficient	1.0	Normal	$\sigma = 0.03$
11	Fuel cladding failure temperature (K)	2500	Normal	$\sigma = 83.3$
12	Molten material drop rate (m/s)	0.5	Normal	$\sigma = 0.017$
13	Debris thermal conductivity multiplier	1.0	Uniform	(0.9, 1.1)
14	Debris specific heat capacity multiplier	1.0	Uniform	(0.9, 1.1)

The parameters of fuel rod air gap size, cladding thickness and internal pressure are closely related to the engineering practice, and errors will inevitably occur in the process of fuel rod manufacturing. According to the processing requirements, these parameters can be considered to follow the normal distribution around the design value. According to the relevant literature [8-10,22] and expert experience, the three parameters of fuel cladding failure temperature, melting drop rate and safe injection water flow all obey normal distribution. For other uncertain input parameters that are not easy to be quantified, it is assumed that they are uniformly distributed within the corresponding range, and each input parameter is generally considered independent of the other.

5. Analysis of Results

5.1. Uncertainty Analysis of Hydrogen Source Term

Assuming that there is a break with an equivalent diameter of 38 mm in the coolant pipeline and the safety injection system is put in place 3000 s after the accident transient. Based on the established serious accident analysis model, SCDAP/RELAP5/MOD3.2 program is used for batch calculation, and then 59 groups of output conditions are analyzed. Figure 8 shows the calculated variation curve of hydrogen production over time. It can be seen that the variation trend of hydrogen production is basically the same.



Figure 8. Hydrogen production of 59 calculation conditions in 38 mm LOCA.

With the input of a safety injection system, the uncertainty of hydrogen production increases obviously. Figure 9 shows the scatter diagram of total hydrogen production under 59 groups of output conditions, and Figure 10 shows the uncertainty range of hydrogen production. It can be seen that different input parameters lead to changes in hydrogen production. Under different output conditions, the minimum hydrogen production of zirconium–water reaction is 20.14 kg, and the maximum is 22.19 kg. It is preliminarily indicated that the uncertain input parameters selected in this paper have a certain influence on the hydrogen production in the pressure vessel.



Figure 9. Scatter diagram of hydrogen production in 38 mm LOCA.



Figure 10. Uncertainty range of hydrogen production in 38 mm LOCA.

5.2. Input Parameter Sensitivity Analysis

Based on the uncertainty analysis of the output results, sensitivity analysis identifies the key parameters that have a great influence on the target parameters by measuring the sensitivity of each input parameter to the target parameters. In statistics, the strength of correlation can be measured by the Spearman correlation coefficient. This coefficient is calculated according to the position ranking of parameter values, which is unrelated to the actual value. The Spearman correlation coefficient is still applicable when the magnitude difference of input parameters is large or a parameter is abnormal without considering the error caused by normalization or other methods. The expression of the Spearman correlation coefficient [26–28] is:

$$\rho_{s} = \frac{\sum_{1}^{n} R_{x_{i}} R_{y_{i}} - n\left(\frac{n+1}{2}\right)^{2}}{\sqrt{\sum_{1}^{n} R_{x_{i}}^{2} - n\left(\frac{n+1}{2}\right)^{2}} \sqrt{\sum_{1}^{n} R_{y_{i}}^{2} - n\left(\frac{n+1}{2}\right)^{2}}}$$
(2)

In the above formula, ρ_s represents the Spearman correlation coefficient, R_{x_i} represents the size ordering of x_i in input variables x, R_{y_i} represents the size ordering of y_i in input variables y, and n represents the number of samples. The value of ρ_s ranges from -1 to 1. The absolute value of ρ_s indicates the strength of the correlation between input parameters and output parameters. The larger the absolute value is, the stronger the correlation is. The sign of ρ_s represents the positive and negative correlation, and $\rho_s > 0$ indicates that the two parameters change into a positive correlation; that is, the output parameter increases with the increase in the input parameter and vice versa.

The calculation results of the Spearman correlation coefficient between the input parameters and hydrogen production are shown in Figure 11 (the corresponding parameters in the figure are the same as those in Table 2).



Figure 11. Spearman rank correlation coefficient of input parameters for hydrogen production in 38 mm LOCA.

The results show that the key input parameter with the greatest influence on hydrogen production is cladding thickness, and its Spearman correlation coefficient is 0.691. This is because the increased thickness of the fuel cladding results in more hydrogen being produced by the zirconium-water reaction. The second-most important input parameter affecting hydrogen production is the safe injection water flow, and its Spearman correlation coefficient is -0.277. After the safety injection system was put in, the coolant entered the core, and then the temperature of the fuel element decreased to inhibit the zirconium-water reaction. Therefore, the greater the safety injection water flow, the less hydrogen was produced. The Spearman correlation coefficient of core resistance is -0.229. The greater the core resistance, the slower the process of coolant entering the core, and the less hydrogen is produced by zirconium-water reaction in the core. The Spearman correlation coefficient of the specific heat capacity of debris is -0.217, and the change in this parameter is negatively correlated with hydrogen production. The larger the specific heat capacity of the migrating debris is, the more heat will be absorbed by the temperature increase at the same mass, which delays the temperature rise rate of other fuels, and then inhibits the zirconium-water reaction and leads to the reduction in hydrogen production. Other uncertain parameters have little influence on the hydrogen source term but also can not be ignored.

6. Conclusions

In this paper, a system and core severe accident analysis model was established for the severe accidents induced by the breaks of marine PWR, and on this basis, it was verified that the established break model could simulate the accident response process of LOCA. The corresponding PIRT was developed for the research object. The established PIRT fills the gap in the uncertainty and sensitivity analysis of severe accidents of marine reactors and provides a reference for subsequent research. Based on the LHS method and Wilks sampling theory, a set of methods for the uncertainty analysis of serious accidents was established. The methods can be applied to the uncertainty and sensitivity analysis of different target parameters.

In this paper, SCDAP/RELAP5/MOD3.2 program was used to complete the uncertainty analysis of hydrogen source terms under severe accidents caused by breaks. In the course of the severe accident analyzed the statistical result of the uncertainty range of hydrogen production from zirconium–water reaction in the pressure vessel was 20.14 kg~22.19 kg with 95% confidence. It could be shown that the selected input parameters had a great influence on hydrogen production. Under the same accident condition, different input parameters had different sensitivities to the target parameters. The Spearman correlation coefficient was used to realize the importance of ranking uncertain parameters. Through the sensitivity analysis of input parameters, it was identified that the fuel cladding thickness had a significant positive correlation with hydrogen production, and its Spearman correlation coefficient was 0.691. Other uncertain parameters were not strongly correlated with hydrogen production, but their importance should not be ignored.

From the perspective of the correlation coefficient, the fuel cladding thickness has a significant effect on hydrogen production, but the actual fuel cladding thickness in the marine reactor is very small, so its engineering error leads to a limited change in the uncertainty of hydrogen production.

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