

Study on Water Chemistry Control Strategy for Ammonia-Containing Primary Loop Coolant

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Abstract

In the primary coolant of specific reactor types, pH is regulated through ammonia addition, and its radiolysis products are utilized to suppress the concentration of oxidizing species, thereby maintaining the reducing state of the coolant. During this process, significant coupled effects exist between ammonia concentration and pH control, necessitating the establishment of a model capable of simulating water chemistry behavior under different control strategies to achieve pH and dissolved hydrogen concentration control. In this work, based on the RETA reactor system analysis code, a model applicable to radiolysis product transport in coolants of arbitrary reactor types was developed; the mean square errors between model predictions and experimental results for NH_3 and H_2 concentrations are only 1.79×10^{-8} and 5.69×10^{-8} , respectively.

Taking the KLT-40S reactor as the object, three ammonia addition control strategies were constructed and comparatively analyzed: initial dispersed ammonia addition, constant-rate source ammonia addition, and constant-rate source ammonia addition based on hydrogen removal optimization. During the simulation process, initial coolant parameters and radiation field conditions were established, with ammonia addition rates and hydrogen removal timing being adjusted progressively. Each strategy was simulated until the system reached quasi-steady state (1.6×10^4 s) to evaluate its control effectiveness on pH and dissolved hydrogen concentration.

The results show that the initial ammonia dispersion strategy is simple and direct, capable of maintaining the reducing state of the system but with a coolant pH control duration of less than 5 h; constant-rate source ammonia addition can effectively regulate coolant pH for extended periods, but introduces the problem of excessively high dissolved hydrogen concentration, requiring a corresponding hydrogen removal scheme. Employing the constant-rate source ammonia addition strategy based on hydrogen removal optimization can simultaneously satisfy

the requirements for stable control of both pH and dissolved hydrogen concentration, with an ammonia addition rate of $1.64 \text{ g} \cdot \text{s}^{-1}$, hydrogen removal device activated 1200 s after ammonia addition commencement, hydrogen removal rate of $0.014 \text{ g} \cdot \text{s}^{-1}$, and after chemical state stabilization, the coolant pH is 6.9 with dissolved hydrogen concentration of $30\text{--}35 \text{ mL} \cdot \text{kg}^{-1}$ (STP).

This work is expected to provide reference for new reactor type development and optimization of water chemistry control strategies.

Full Text

Preamble

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Study on Water Chemistry Control Strategy for Ammonia-Containing Coolant in the Primary Circuit

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Abstract

[Background] In certain reactor types, ammonia is added to the primary coolant to regulate pH, and its radiolytic products are utilized to suppress the concentration of oxidizing species, thereby maintaining the coolant in a reductive state. During this process, ammonia concentration and pH regulation exhibit significant coupling effects, necessitating the development of a model capable of simulating water chemistry behavior under different control strategies to achieve coordinated control of both pH and dissolved hydrogen concentration. **[Purpose]** This study aims to develop a predictive model for simulating water chemistry behavior under various control strategies. **[Methods]** A transport model for radiolytic species in reactor coolant applicable to arbitrary reactor types was developed based on the RETA reactor system analysis code. The model demonstrated high predictive accuracy, with root-mean-square errors of only 1.79×10^{-8} for NH_3 and 5.69×10^{-8} for H_2 concentrations compared with experimental data. Using the KLT-40S reactor as a case study, three ammonia injection strategies were established and comparatively evaluated: initial dispersion, constant-rate injection, and constant-rate injection optimized with hydrogen removal. Simulations were conducted by defining initial coolant parameters and radiation field conditions, followed by stepwise adjustment of ammonia injection rates and hydrogen removal timing. Each strategy was simulated until the system reached quasi-steady state (1.6×10^4 s) to assess

its effectiveness in controlling pH and dissolved hydrogen levels. **[Results]** The results indicated that the initial dispersion strategy, while straightforward and effective in maintaining a reductive environment, could sustain pH regulation for less than 5 hours. The constant-rate ammonia injection strategy enabled long-term pH control but resulted in excessive dissolved hydrogen concentrations, requiring a corresponding hydrogen removal scheme. The hydrogen removal-optimized constant-rate injection strategy successfully met the requirements for stable control of both pH and dissolved hydrogen concentration, with an ammonia injection rate of $1.64 \text{ g} \cdot \text{s}^{-1}$, hydrogen removal initiated 1200 s after ammonia injection began at a rate of $0.014 \text{ g} \cdot \text{s}^{-1}$, achieving a stable coolant pH of 6.9 and dissolved hydrogen concentration of $30\text{--}35 \text{ mL} \cdot \text{kg}^{-1}$ (STP). **[Conclusions]** This work is expected to provide valuable reference for the development of new reactor types and optimization of water chemistry control strategies.

Keywords: Coolant, Reactor, Ammonia, Radiolysis, Water chemistry

Small Modular Reactors (SMRs) offer promising applications in specialized fields such as icebreakers and floating nuclear power plants due to their compact structure, light weight, and flexible deployment. However, the highly integrated and compact design of SMR loop systems imposes more stringent requirements on radiation protection and material service safety compared to conventional reactors [1,2]. In particular, the generation and accumulation of radiolytic products, such as reactive species including oxygen (O_2) and hydrogen peroxide (H_2O_2), may adversely affect system chemical stability and operational safety [3-5]. Therefore, to deeply understand the generation mechanisms of radiolytic products and their migration and transformation behavior in the coolant system, it is essential to obtain accurate thermal-hydraulic parameters and couple them closely with water chemistry processes to achieve comprehensive analysis of radiochemical effects in SMR coolant systems.

The issue of irradiation in reactors has long been recognized [6-8]. Scott's research demonstrated that, in addition to direct radiation damage to materials, coolant radiolysis is a key factor causing material corrosion [9]. Radiolysis refers to the production of various chemical species in water within the core region under high-flux neutron and gamma radiation [10,11]. Water chemistry issues primarily focus on the generation, transport, and reaction behavior of these radiolytic products. While most products have extremely short lifetimes, some relatively stable species (such as H_2O_2 and O_2) can persist in the system and potentially degrade water quality [11,12]. As these oxidizing species migrate through the primary circuit, they may cause severe oxidative corrosion, particularly threatening critical thin-walled structures such as stainless steel heat exchanger tubes [13]. Recently, Sultana et al. conducted experimental studies on radiolysis effects in supercritical water (SCW) and noted that similar issues may exist in SMR systems [14].

Since water chemistry issues have received widespread attention, the radiolysis

process of coolant has been extensively studied. Ershov et al. first proposed and validated a kinetic model for pure water radiolysis, systematically describing the generation mechanisms of major radiolytic products including H_2 , H_2O_2 , and O_2 [15]. Subsequently, Joseph et al. further investigated radiolysis effects in pure water through numerous experiments and developed a kinetic model for predicting the generation behavior of multiple products [16]. Elliot compiled and reported 60 key radiolytic reactions and their rate constants, providing an important foundation for water chemistry simulation calculations [17].

Subsequent research has focused on achieving better agreement with experimental results and broader simulation scope. Yakabuskie introduced mass transfer processes at two-phase interfaces to modify and improve the model based on Joseph's work [18]. Palfi investigated the generation processes and yields of transient products in aqueous solutions under pulse irradiation conditions using a combination of experimental and computational methods [19]. Karditsas studied water radiolysis in ITER fusion reactors, proposing a time-dependent transport model and providing calculation examples [20]. Yousefi extended the application scope of radiolysis models to high-temperature and high-pressure conditions, providing a theoretical basis for analyzing radiolysis behavior under more complex operating conditions [21].

Another research focus has been on influencing factors and control strategies for radiolytic products. Roth and Daub analyzed the effect of pH on H_2O_2 generation and carbon steel corrosion behavior [22,23]. Dey reviewed the transformation processes of nitrogen-containing substances in aqueous solutions under irradiation conditions, proposing that NH_3 has the potential to regulate oxidizing species and providing a new possible means for corrosion control [24]. Building on this, Yakabuskie studied the radiolysis behavior of NO_3^- and NO_2^- solutions [25], while Guo analyzed the radiolysis process of ammonia water under different influencing factors [26]. Kumar evaluated the role of N_2H_4 in corrosion control [27], and Iwamatsu studied the effect of H_2 in suppressing H_2O_2 accumulation [28].

The aforementioned work has primarily focused on homogeneous zero-dimensional systems, neglecting spatial distribution effects and lacking guidance for loop analysis. Considering that radiolytic products are generated in the core and transported through the primary circuit, mass, momentum, and energy equations can be combined to calculate the concentration evolution of products. In this work, integrating research in radiation chemistry, thermal-hydraulics, and numerical computation, a model was developed to simulate the coupled thermal-hydraulic and water chemistry effects in SMRs. This model is based on the RETA system analysis code with an added submodule for water chemical reactions and transport. The model's reliability and performance were subsequently verified and evaluated, and the primary circuit of the KLT-40S reactor was modeled to analyze the control effectiveness and advantages/disadvantages of two ammonia injection strategies. This work is expected to provide reference for optimizing ammonia-containing water

chemistry control strategies.

1.1 Radiolysis Process

The radiolysis process can be summarized in three stages: (1) radiation deposits energy in the coolant, leading to the production of a series of excited species such as H_2O^* , H_2O^+ , and e^- ; (2) excited species react to generate intermediate products such as $\cdot\text{H}$ and $\cdot\text{OH}$ radicals; and (3) excited species and intermediate products react with each other to form final radiolytic products that diffuse out of the spur, such as H_2O_2 , O_2 , and H_2 (as shown in R0).

For zero-dimensional calculations of coolant radiolysis, the dose rate of radiation can be converted into a source term for radiolytic product generation by introducing G-values. The radiolytic production rate $S_{i,r}$ ($\text{mol} \cdot \text{L}^{-1} \cdot \text{s}^{-1}$) for species i is defined as:

$$S_{i,r} = \frac{\rho D_r G_i N_A}{100}$$

where ρ represents the coolant density ($\text{kg} \cdot \text{L}^{-1}$), e is the electron charge ($1.9 \times 10^{-19} \text{ C}$), G_i is the radiation chemical yield of species i (/100 eV), D_r is the absorbed dose rate ($\text{Gy} \cdot \text{s}^{-1}$), and N_A is Avogadro's constant ($6.02 \times 10^{23} \text{ mol}^{-1}$).

Under continuous irradiation, various species react with each other. For species i , which is continuously generated and consumed during radiolysis, the net generation can be expressed by Equation E2:

$$\frac{dC_i}{dt} = S_{i,r} + \sum_{s=1}^N \sum_{m=1}^M k_{sm} C_s C_m - \sum_{s=1}^N k_{si} C_s C_i$$

where k_{sm} and k_{si} are rate constants for reactions between species s and m (generating i) or between s and i (consuming i), respectively; C_m , C_s , and C_i are concentrations of species m , s , and i ; N is the total number of reactions; and M is the number of species involved in the reactions.

1.2 Thermal-Hydraulic Model

For engineering applications, zero-dimensional radiolysis calculations are insufficient and should be extended to at least the primary circuit and its main components. This requires coupled thermal-hydraulic and mass transfer calculations in addition to radiolytic reactions. The simplified primary circuit model and mesh division used in this paper are shown in [Figure 1: see original paper].

For numerical solution of the equations and integration of radiation chemistry into reactor analysis, programming was performed based on the RETA software

from the University of Science and Technology of China, employing the fully implicit numerical discretization method of the Finite Volume Method (FVM). The control equations were solved using the Preconditioned Jacobian-Free Newton-Krylov (PJFNK) algorithm. Based on RETA, an additional module called R-WRC was developed, focusing on radiolysis calculations and capable of coupling with RETA's core thermal-hydraulic functions. The implementation in R-WRC involves direct programming to include transport terms:

$$\frac{\partial \mathbf{C}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{C}) = \nabla \cdot (\mathbf{D}\nabla \mathbf{C}) + \mathbf{S}_r + \mathbf{S}_c$$

where \mathbf{C} is the species concentration vector, \mathbf{u} is the local velocity vector, \mathbf{D} is the diffusion coefficient for different species, \mathbf{S}_r is the source term from radiation-induced products, and \mathbf{S}_c is the collection of chemical reactions.

Parameters such as \mathbf{u} and \mathbf{D} are crucial in thermal-hydraulic calculations. To simplify the coupling of radiolysis with thermal-hydraulics, the following assumptions were made:

1. Only one-dimensional equations are considered, corresponding to the one-dimensional mesh in RETA system thermal-hydraulic simulations, similar to RELAP;
2. Diffusion terms are neglected, as velocities in the main loop are sufficiently high to ignore species diffusion processes.

Based on these two assumptions, the simplified equation becomes:

$$\frac{\partial \mathbf{C}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{C} = \mathbf{S}_r + \mathbf{S}_c$$

Due to the large number of mesh nodes that need to be considered in the solution process, making it extremely challenging, the following programming structure was established: (1) process each species at all mesh nodes individually; (2) combine all species into a unified vector; and (3) use a large sparse matrix.

1.3 Model Validation

To verify the reliability of the R-WRC module in radiolysis calculations, its results were compared with simulation data from the specialized radiochemistry software FACSIMILE, as shown in [Figure 2: see original paper]. Both R-WRC and FACSIMILE were used to simulate the radiolysis behavior of aqueous ammonia solutions with initial concentrations of 1-3 mol · L⁻¹ at 25 °C, and the variations of H⁺ concentration (pH), ammonia concentration, and N₂ concentration with irradiation time were compared and analyzed.

The results demonstrate that R-WRC can accurately describe the radiolysis process, with minimal differences between its simulation results and FACSIMILE, showing good computational accuracy and reliability.

To further validate the model's reliability, radiolysis experiments were conducted using aqueous ammonia solutions with an initial concentration of $30 \text{ mg} \cdot \text{L}^{-1}$, which were continuously irradiated for 72 h. The measured changes in NH_3 and H_2 concentrations were compared with simulation results, as shown in [Figure 3: see original paper]. The simulated values for NH_3 and H_2 agree well with the experimental data, with mean square errors (MSE) of only 1.79×10^{-8} and 5.69×10^{-8} , respectively, indicating high accuracy in describing the main reaction pathways and radiolytic product generation during the experiment affecting the system's acidity.

In summary, the model established in this work can effectively predict the evolution of major radiolytic products during ammonia solution radiolysis with high accuracy.

2 Model Establishment and Validation

The objective of primary circuit water chemistry control is to ensure the integrity of the primary circuit pressure boundary, fuel cladding integrity, and achievement of fuel design performance, while minimizing the ex-core radiation field level as much as possible. The core control strategy is to maintain the coolant pH and dissolved hydrogen concentration within acceptable ranges, thereby ensuring the coolant remains in an alkaline and reductive environment. For conventional PWRs using boron-lithium coordinated control, the pH during operation is typically controlled between 6.9 and 7.2, corresponding to OH^- concentrations of approximately 10^{-5} - $10^{-6} \text{ mol} \cdot \text{L}^{-1}$; dissolved hydrogen concentration is usually maintained within the range of 2-4.5 $\text{mg} \cdot \text{L}^{-1}$.

2.1 Simulation of Initial Dispersion Ammonia Injection Strategy

The initial dispersion ammonia injection strategy refers to injecting a given amount of ammonia solution into the primary circuit at the start of system operation, allowing it to rapidly disperse and achieve uniform mixing throughout the coolant system. In the model, this is implemented by assigning the same initial ammonia concentration to all mesh nodes to simulate its uniform distribution in the system. As core irradiation continues and coolant circulates through the loop, species in each mesh node are continuously transported and updated, with their concentrations dynamically changing due to reaction and transport processes, showing time-dependent evolution.

To investigate the effects of different initial ammonia dispersion concentrations, the model was used to calculate the time-dependent changes in H_2 and OH^- concentrations during radiolysis of ammonia-containing coolant at concentrations of 0-100 $\text{mg} \cdot \text{L}^{-1}$. The 0 $\text{mg} \cdot \text{L}^{-1}$ pure water radiolysis data served as the control group, 5 and 10 $\text{mg} \cdot \text{L}^{-1}$ as low concentration levels, 17, 34, and 51 $\text{mg} \cdot \text{L}^{-1}$ as medium concentration levels, and 60, 80, and 100 $\text{mg} \cdot \text{L}^{-1}$ as high concentration groups. To evaluate the chemical effects caused by the slow depletion of

ammonia during long-term reactor operation and to observe the establishment of concentration steady state, the simulation time was set to 1.6×10^4 s, with results shown in [Figure 4: see original paper].

[FIGURE:4(a)] shows that H_2 concentration quickly reaches chemical steady state with irradiation, and increasing the initial ammonia dispersion concentration significantly enhances H_2 generation rates. At an irradiation time of 1.6×10^4 s, the H_2 concentration in the $0 \text{ mg} \cdot \text{L}^{-1}$ system is approximately $0.02 \text{ mg} \cdot \text{L}^{-1}$, low ammonia concentration groups show $0.62\text{--}1.25 \text{ mg} \cdot \text{L}^{-1}$, medium ammonia groups show $2.12\text{--}6.34 \text{ mg} \cdot \text{L}^{-1}$, and the high ammonia concentration group ($100 \text{ mg} \cdot \text{L}^{-1}$) reaches $12.36 \text{ mg} \cdot \text{L}^{-1}$. These results indicate that the medium concentration dispersion strategy with initial ammonia concentrations of 17 and $34 \text{ mg} \cdot \text{L}^{-1}$ can meet the H_2 limit requirements, while both low and high concentration groups fail to satisfy the requirements.

From the coolant pH perspective, all ammonia dispersion strategies fail to maintain an alkaline state for extended operation times, as shown in [FIGURE:4(b)]. After initial ammonia addition and irradiation start, the coolant pH rapidly decreases, falling from weakly alkaline to neutral (at 280°C) within 1–5 h, and eventually approaching neutral levels within 24 h. It should be noted that while short-term pH changes may not directly accelerate material corrosion, the loss of alkaline environment may induce more unfavorable corrosion tendencies for metallic materials, posing potential risks in actual reactor operation.

In summary, the initial dispersion ammonia injection strategy can maintain dissolved hydrogen concentration within the target limit range by controlling ammonia concentration between $17\text{--}34 \text{ mg} \cdot \text{L}^{-1}$. However, due to the difficulty in maintaining alkaline conditions long-term, with system pH rapidly falling back to neutral after irradiation begins, this strategy cannot simultaneously achieve the two major goals of coolant chemistry control: meeting dissolved hydrogen concentration requirements and maintaining a weakly alkaline environment.

2.2 Simulation of Constant-Rate Ammonia Injection Strategy

Since the initial dispersion strategy cannot meet primary circuit water chemistry control requirements, a constant-rate ammonia injection strategy was adopted to achieve long-term stable pH control in the coolant system. This involves applying a stable ammonia source term before coolant enters the core to simulate the continuous ammonia injection effect of the chemical volume control system in the primary circuit. Compared with initial dispersion, this strategy can maintain relatively stable ammonia concentration in the core over longer periods. This section calculates the evolution of dissolved hydrogen and OH^- concentrations under continuous ammonia injection rates of $0\text{--}16.4 \text{ g} \cdot \text{s}^{-1}$ at the core inlet and under square-wave intermittent injection at $1.64 \text{ g} \cdot \text{s}^{-1}$, with results shown in [Figure 5: see original paper].

[FIGURE:5(a)] shows that under the constant-rate injection strategy, excessive injection rates can easily cause dissolved hydrogen concentration to rapidly exceed the limit range. For example, at an injection rate of $1.64 \text{ g} \cdot \text{s}^{-1}$, H_2 concentration exceeds $20 \text{ mg} \cdot \text{L}^{-1}$ at 8000 s, far above the upper limit. Even at lower injection rates ($0.164 \text{ g} \cdot \text{s}^{-1}$), H_2 concentration may exceed limits if irradiation time is sufficiently long. Although stopping injection can suppress further H_2 accumulation, the concentration does not quickly return to the normal range and may instead increase further due to continued radiolysis of residual ammonia in the system. These results indicate that the constant-rate injection strategy carries potential risks of H_2 concentration exceeding limits.

Improvements were made to the constant-rate injection strategy by attempting square-wave intermittent injection, i.e., injecting ammonia at $1.64 \text{ g} \cdot \text{s}^{-1}$ for 1 h, stopping for 1 h, and repeating this cycle. Simulation results show that this improved strategy still carries the risk of dissolved hydrogen concentration exceeding limits within a relatively short time (approximately 2000 s). Although pH can be maintained relatively stable initially, as shown in [FIGURE:5(b)], the cumulative effect of ammonia in the system with increasing cycles may cause pH to continuously rise, posing potential overrun risks.

Additionally, as shown in [FIGURE:5(b)], compared with continuous constant-rate injection, square-wave intermittent injection offers stronger pH controllability. The former only shows pH controllability within a short time at injection rates of 0.164 and $1.64 \text{ g} \cdot \text{s}^{-1}$, while both too low ($0.0164 \text{ g} \cdot \text{s}^{-1}$) and too high ($16.4 \text{ g} \cdot \text{s}^{-1}$) rates cannot effectively control coolant pH.

In summary, square-wave intermittent injection has certain effectiveness in pH control, allowing system pH to fluctuate within the target range by adjusting injection frequency and concentration. However, regardless of the control method, H_2 concentration risks exceeding limits, making it difficult for this ammonia injection strategy to fully meet established water chemistry control objectives. To address the continuous H_2 concentration increase under this strategy, hydrogen removal measures can be further introduced to simulate their effectiveness in controlling H_2 concentration and achieve comprehensive optimization of water chemistry status.

2.3 Simulation of Hydrogen-Removal-Optimized Constant-Rate Ammonia Injection Strategy

Since both initial dispersion and constant-rate injection strategies have limitations, this section introduces a hydrogen removal mechanism based on the constant-rate injection strategy. For injection rates of 0.164 and $1.64 \text{ g} \cdot \text{s}^{-1}$, corresponding hydrogen removal rates were matched ($0.164 \text{ g} \cdot \text{s}^{-1}$ injection: $-0.00148 \text{ g} \cdot \text{s}^{-1}$ removal; $1.64 \text{ g} \cdot \text{s}^{-1}$ injection: -0.0140 , -0.0150 , $-0.0160 \text{ g} \cdot \text{s}^{-1}$ removal). The hydrogen removal process was simulated by setting a negative H_2 source term at the top of the meshed core region. It should be noted that earlier activation of the hydrogen removal device leads to lower steady-state levels of

both hydrogen concentration and pH, while later activation results in higher steady-state levels. Since the initial H_2 concentration in the coolant system is zero, to avoid calculation errors and based on comprehensive consideration of pH control after ammonia injection and hydrogen removal rate, this negative source term was set to activate after reaching specific times (1200 s, 10800 s). Simulation results are shown in [Figure 6: see original paper].

[FIGURE:6(a)] shows that higher hydrogen removal rates cause dissolved hydrogen concentration to drop rapidly, potentially leading to adverse consequences such as oxygen removal failure. For example, under $1.64 \text{ g} \cdot \text{s}^{-1}$ ammonia injection, when removal rates are 0.016 and $0.015 \text{ g} \cdot \text{s}^{-1}$, H_2 concentration falls to the lower limit at approximately 2000 s and 7200 s, respectively. In contrast, appropriately reducing the removal rate (e.g., to $0.014 \text{ g} \cdot \text{s}^{-1}$) can maintain H_2 concentration within a reasonable range. Similarly, at lower injection rates ($0.164 \text{ g} \cdot \text{s}^{-1}$), further reducing the removal rate ($-0.00148 \text{ g} \cdot \text{s}^{-1}$) also helps achieve H_2 concentration compliance.

pH variations are shown in [FIGURE:6(b)]. In constant-rate injection strategies without hydrogen removal, pH continuously increases with irradiation time, eventually exceeding the upper pH limit. At $1.64 \text{ g} \cdot \text{s}^{-1}$ injection with 0.016 and $0.015 \text{ g} \cdot \text{s}^{-1}$ removal rates, pH can only be maintained for 2 and 4 h, respectively. Further analysis of two ammonia injection strategies meeting H_2 concentration requirements reveals that both can satisfy pH limit ranges, with the general principle that lower ammonia injection rates result in lower hydrogen removal pressure and lower steady-state pH and dissolved hydrogen levels.

In summary, through hydrogen removal optimization studies of the constant-rate injection strategy, two reasonable control schemes were obtained:

1. Constant-rate ammonia injection at $1.64 \text{ g} \cdot \text{s}^{-1}$, with hydrogen removal device activated 1200 s after injection begins at a removal rate of $0.014 \text{ g} \cdot \text{s}^{-1}$, corresponding to $\text{pHT} = 6.9$;
2. Constant-rate ammonia injection at $0.164 \text{ g} \cdot \text{s}^{-1}$, with hydrogen removal device activated 10800 s after injection begins at a removal rate of $0.0014 \text{ g} \cdot \text{s}^{-1}$, corresponding to $\text{pHT} = 6.5$.

Both schemes yield dissolved hydrogen concentrations of approximately $2.7\text{--}3.1 \text{ mg} \cdot \text{L}^{-1}$, i.e., $30\text{--}35 \text{ mL} \cdot \text{kg}^{-1}$ (STP). However, considering that higher coolant pH can more effectively reduce corrosion of metallic materials in the primary circuit system, the first scheme is superior.

This paper established a water chemistry control model for ammonia-containing coolant in the primary circuit and studied the radiolysis behavior of ammonia-containing coolant using the KLT-40S reactor as an example. The effects of initial dispersion injection, constant-rate injection, and hydrogen-removal-optimized constant-rate injection strategies on dissolved hydrogen and pH were compared. The results show that: (1) the initial dispersion strategy can achieve dissolved hydrogen concentration compliance and maintain coolant reductive control but cannot effectively regulate coolant pH; (2) the constant-rate injection

tion strategy has shortcomings in dissolved hydrogen concentration control, and while square-wave intermittent injection can achieve pH regulation, it cannot maintain dissolved hydrogen concentration within limits for extended periods; (3) the hydrogen-removal-optimized constant-rate injection strategy can simultaneously achieve coolant pH regulation and dissolved hydrogen concentration control by matching appropriate hydrogen removal rates; and (4) a reasonable water chemistry control scheme is provided: ammonia injection rate of $1.64 \text{ g} \cdot \text{s}^{-1}$, hydrogen removal initiated 1200 s after injection begins at a removal rate of $0.014 \text{ g} \cdot \text{s}^{-1}$.

Author Contributions

LUO Tianjun, YUAN Yukun: Code development, data analysis, and manuscript drafting

ZHOU Xiaoyuan: Data processing

GUO Zifang: Manuscript revision and final proofreading

DU Yingzhe, LIN Peng: Research platform provision and funding acquisition

HU Guojun: Quality review and content oversight

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