BAYESIAN OPTIMIZATION ANALYSIS OF CONTAINMENT VENTING OPERATION IN A BWR SEVERE ACCIDENT

Xiaoyu Zheng[1], Jun Ishikawa[1], Tomoyuki Sugiyama[1], Yu Maruyama[1]

[1] *Japan Atomic Energy Agency, 2-4, Shirakata, Tokai-mura, Naka-gun, Ibaraki-ken 319-1195, Japan,*
zheng.xiaoyu@jaea.go.jp, ishikawa.jun@jaea.go.jp, sugiyama.tomoyuki@jaea.go.jp, maruyama.yu@jaea.go.jp

After the occurrence of a nuclear power plant severe accident, the release of fission products can be mitigated by severe accident management measures. Containment venting is one of essential measures to protect the integrity of the final barrier of a nuclear reactor, by which the uncontrollable release of fission products can be avoided. The authors seek to develop an optimization approach, and then apply it, from a simulation-based perspective, to the planning of containment-venting operations by using an integrated severe accident code, THALES2/KICHE. Factors that control the activation of the venting system, for example, the containment pressure, the amount of fission products within the containment and pH value in the suppression chamber water pool, will affect the radiological consequences. The effectiveness of containment venting strategies needs to be confirmed through numerical simulations via computer codes with the setting of venting-related factors. The number of iterations, however, needs to be controlled for cumbersome computational burden of severe accident codes, especially when many factors need to be taken into account. Bayesian optimization is a computationally efficient global optimization approach to find desired solutions. With the use of Gaussian process regression, a surrogate model of the "black-box" code is constructed, and it can be updated simultaneously whenever more simulation results have been acquired. According to the predictions through the surrogate model, the upcoming location of the most probable optimum can be revealed. The sampling procedure is so-called adaptive. The number of code queries is largely reduced for the optimum finding, compared with simpler methods such as pure random (Monte Carlo) search or grid search. One typical severe accident scenario of a boiling water reactor (BWR) is chosen as an example of analysis. The research demonstrates the applicability of the Bayesian optimization approach to the design and establishment of containment-venting strategies under BWR severe accident conditions.

Keywords: Severe accident, containment venting, THALES2/KICHE code, fission products, Bayesian optimization, Gaussian process, adaptive sampling

I. INTRODUCTION

The establishment of strategies in response to severe accident conditions is fraught with enormous choices, usually with the involvement of many academic disciplines and influential factors. Effective severe accident management measures can ensure the prevention of reactor core damage, containment vessel failure, and/or the final mitigation of radiological consequences. Because of the complexity, the most decisions for severe accident management measures are mainly made by expert judgements at present. Mathematically, the optimization of the design of a specific accident countermeasure can be converted to an equivalent task of finding the optimal solution of an objective function[1]. When the objective function has no explicit form, especially in many engineering fields, it is called a "black-box" objective function, such as an integral severe accident code or an experimental facility. The only way to get corresponding outputs of the "black-box" function is to evaluate it, and it usually needs computational/practical effort, sometimes too expensive to be unaffordable. To overcome the inefficiency of random or grid search for the optimal solution, we can adopt methods of deterministic global searching[2] or stochastic methods using the Bayesian theory[3]. A simulation-based framework using the latter approach has been proposed, and then, as a demonstration, the containment venting operation under a boiling water reactor (BWR) severe accident condition is optimized to reduce the total release of fission products from the containment of a nuclear reactor. To simplify the problem, the venting system analyzed is without the installation of any filter. The outputs from the present optimization analysis are equivalent to the amount of fission products introduced into a filtered venting system.

In general, BWR containments use suppression chambers (S/Cs), also known as wetwells, to condense water vapor. When under severe accident scenarios, venting of a containment vessel might be required to prevent containment failure resulting from overpressure by removing steam, hydrogen and other gases[4]. One primary requirement in Order EA-13-109, issued by the U.S. Nuclear Regulatory Commission, is that Mark I and Mark II containments must have S/C venting systems that remain functional during severe accident conditions[5]. The establishment of containment-venting activation rules directly affects the containment integrity, and likewise the environmental fission product releases. The venting operations are affected by, for example, the timing of activation/deactivation and the duration of each phase. The problem is complex and affected by many factors. When containment venting rules are designed, the effectiveness of them to containment protection and consequence mitigation needs to be inspected. To find the optimal setting of these influential factors, with the minimization of the fission product release, queries via computer simulations, using integrated severe accident codes, are required.

Japan Atomic Energy Agency (JAEA) has been developing the THALES2 code to analyze the severe accident progression and estimate source terms for Level 2 probabilistic risk assessment[6]. In recent years, an independent computer code of iodine chemistry simulation, KICHE[7,8], has been coupled with THALES2, through an interface program developed for the exchange of input/output between two codes[9]. THALES2/KICHE is an integrated and fast-running severe accident code, which simulates the progression of severe accidents in light water reactor nuclear power plants, including simplified modeling of thermal-hydraulic response, core melt progression, and in-vessel and ex-vessel transport behavior of radioactive materials with the consideration of iodine chemical reaction kinetics in aqueous phase, etc.

The paper is organized as follows. In Section 2, we describe the analysis of a typical BWR severe accident using the THALES2/KICHE code. In Section 3, we demonstrate the Bayesian optimization framework. In Section 4, the venting strategy is optimized under severe accident conditions to mitigate the radioactive releases from the containment vessel.

II. SEVERE ACCIDENT ANALYSIS VIA THALES2/KICHE

The BWR4 plant model with a Mark I containment is discretized with control volumes as shown in Fig. 1. The reactor cooling system is divided into seven volumes, consisting of reactor core, upper plenum, steam dome, downcomer, lower plenum and recirculation loops A and B. The containment vessel model comprises drywell (D/W), suppression chamber (S/C), pedestal and vent pipes that connect D/W and S/C. The environment volume is connected to the reactor building and S/C, which represent paths of the containment leak and S/C vent.

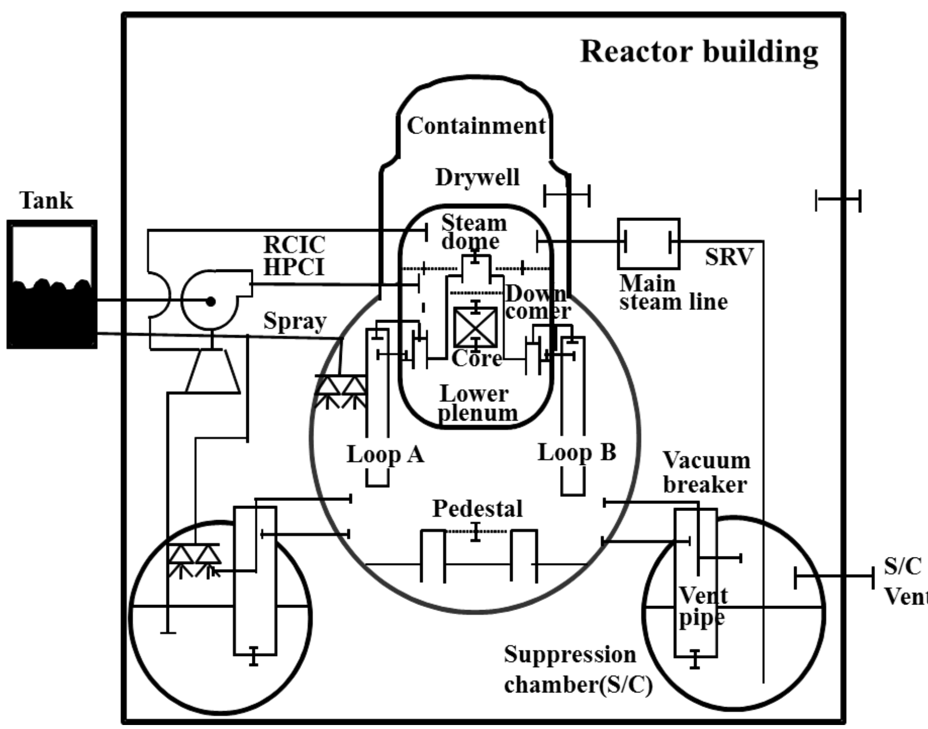

Fig. 1. Control volume nodalization for THALES2/KICHE modeling

After a severe accident occurs, fission products released from a degraded core could transcend the reactor cooling system, containment, and reactor building. During then, vigorous physical and chemical processes take place and the fission products are drastically transformed[10]. The activation timing and duration of venting system are quite crucial for the consequence mitigation: less fission products would be released if the concentration of in-containment gaseous radionuclides is low and filtering function of S/C works favorably; otherwise, more fission products would be released. The transportation and release of representative fission products are simulated by using the THALES2/KICHE code, and it will be discussed about how to establish the effective venting operations.

As an example, one of typical BWR severe accident sequences[11], TQUV (a transient (T) followed by failure of feedwater system (Q), high pressure coolant injection system (U) and low pressure coolant injection system (V) with depressurization of reactor coolant system), is chosen to demonstrate the current approach of global optimization. Immediately after the occurrence of the transient, the reactor is scrammed and successfully depressurized. Upon the loss of coolant injection, the vessel water level starts to decrease because of the coolant inventory loss in the form of steam. Afterwards, excess vessel pressure is relieved through safety relieve valves (SRV) lines and steam discharges into the S/C. Finally, with the continuing loss of coolant, core melt progression starts and more fission products are released with the steam and hydrogen to the water pool in S/C. Fission products such as cesium and iodine are at first scrubbed in the water pool. The dissolved iodine can be transformed into volatile species, such as molecular iodine and organic iodine, according to aqueous phase iodine chemistry. A significant amount of volatile fission products are then released from the water, and finally out of the containment via venting or probable leak paths. The amount of fission product release is largely dependent on the pH value of the water pool.

One key to controlling the amount of radioactive material released from containment is minimizing the airborne amount in the containment, including D/W and S/C, during venting[1]. From points of view on the formation and release of volatile iodine, the pH value in the S/C water pool is taken into account in the present analysis as another key to controlling the radioactive material releases although the corresponding measurement is not currently made for it. Important factors also include the opening and closing pressures for venting operations. To simplify the current study, let us focus on the four most important factors, and build a model to minimize the fission product releases from the containment. The definition and notation of each factor are summarized in Table 1.

Table 1. Factors selected for the establishment of venting rules

Notation	**Factor Description**
x_1	Pressure (forced open): when the containment pressure is higher than x_1, the S/C vent is forcedly activated for depressurization.
x_2	Pressure (conditional open): when the containment pressure is higher than x_2, total amount of fission products in D/W and S/C is less than x_3, and pH value in S/C is higher than x_4, the S/C vent is switched on for depressurization.
x_3	In-containment fission products mass criterion (D/W and S/C)
x_4	The pH value criterion (S/C pool)
x_5 (fixed)	Pressure (forced close): when the containment pressure is less than this value, the S/C venting is forcedly deactivated.

As the input vector is determined as $\mathbf{x} = \left[x_1, x_2, x_3, x_4\right]^T$, the optimization of venting operation is converted into the mathematical optimization problem as to find the $\mathbf{x}^*$ minimizing the fission product release, which can be written as an objective function, $f\left(\mathbf{x}\right)$. Before the solving of the optimization of containment-venting operations, let us review the Bayesian global optimization with a simple example.

III. BAYESIAN OPTIMIZATION WITH A GAUSSIAN PROCESS REGRESSION MODEL

The problem of finding a reliable venting strategy, which means to control the release of fission products to a minimal level, can be converted to minimize an unknown or “black-box” function:

$$\mathbf{x}^* = \underset{\mathbf{x}\in \mathrm{X}}{\arg\min}\, f\left(\mathbf{x}\right) \tag{1}$$

Here, $f\left(\cdot\right)$ is the objective function, with respect to the controlling inputs $\mathbf{x}\in \mathrm{X}$, and $\mathbf{x}^*$ is the specific input we try to find, which minimize the response of the objective function $f\left(\cdot\right)$. In severe accident analysis, the objective function $f\left(\cdot\right)$

can be equivalently treated as the computer code, THALES2/KICHE, and hence we need to query the function value at arbitrary $\mathbf{x} \in \mathrm{X}$ through an execution of the code.

The optimization algorithm should quickly find local optimums while easily jump out to other area for finding next local/global optimum, and it is called the tradeoff of “exploitation” and “exploration”. The “exploitation” promotes the search in “more interested” area where local optimums locate, and the “exploration” promotes the search in “more potential” area. More introduction of Bayesian optimization can be found in references[12-14]. In the paper, we provide the introduction from the perspective of a surrogate model[15,16]. Within the Bayesian framework, since the objective function is unknown, the tactic is to treat it as a random function, which we named as a surrogate model, and place a prior distribution over it. After any evaluations of the objective function are performed, the gathered data can be used to update the prior function to a posterior function. The posterior function, in turn, can provide us useful information for the prediction of next possible optimum. The procedure of Bayesian optimization with a surrogate model is illustrated in Fig. 2. Thus the selection of different surrogate models leads to different scheme of Bayesian optimization. Mainly, when the output space is continuous, there are two main suites of models: parametric (such as linear and generalized linear models) and nonparametric (such as Gaussian process regression) models. We also named the method as an adaptive sampling method since the choice of input is guided by the surrogate model.

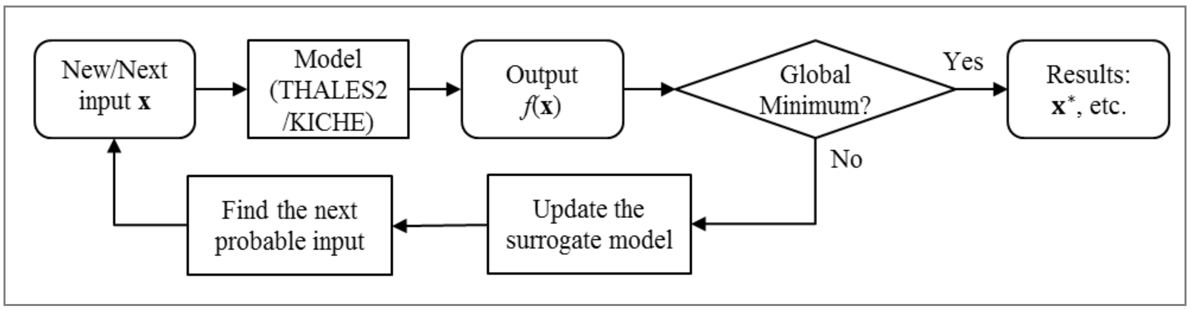

Fig. 2. The adaptive-sampling procedure of Bayesian optimization

In the paper, we apply the Gaussian process regression to construct a surrogate model of the THALES2/KICHE code. Gaussian process can be used as a prior probability distribution over functions in Bayesian inference[17,18]. The Bayesian update over the function space can be written as

$$p\left(\tilde{f}\,|D\right) = \frac{p\left(\tilde{f}\right)p\left(D\middle|\tilde{f}\right)}{p\left(D\right)} \tag{2}$$

Here, $\tilde{f}$ denotes the predictive function over the input space, so $p\left(\tilde{f}\right)$ is the prior distribution of the predictive function, and $p\left(\tilde{f}\,|D\right)$ is the posterior distribution of the predictive function after a number of data or simulation results in this paper, D, are gathered. $p\left(D\middle|\tilde{f}\right)$ is the likelihood function. $p\left(D\right)$ is the marginal likelihood. If the input space is discretized, for the simplest example as a one-dimensional model, the obtained $\mathbf{x}_1 = \left(x_1^{(0)}, x_1^{(1)}, x_1^{(2)}, \ldots, x_1^{(n)}\right)^T$ follows a multivariate Gaussian distribution, and it is defined as a Gaussian process (GP). The predictive function can be written as

$$\tilde{f} \sim GP\left(m, k\right) \tag{3}$$

The Bayesian update of Eq. (2) converts to the update of the mean function, $m\left(x\right)$, and the covariance function, $k\left(x, x^{'}\right)$, both of which are written in the scalar form. As the multivariate Gaussian distribution is conjugate to itself, the posterior distribution of responses over the discretized input space can correspondingly be given by an updated multivariate Gaussian distribution. In the following parts, the bold uppercase **X** denotes an input matrix, and the bold lowercase **x** denotes an input vector.

$$\mathbf{f}^* \left| D, \mathbf{X}^* \sim N\left(\boldsymbol{\mu}\left(\mathbf{X}^* | D\right), \boldsymbol{\Sigma}\left(\mathbf{X}^* | D\right)\right)\right. \tag{4}$$

Here, the dataset can equivalently be written as $D = \{\mathbf{X}, \mathbf{f}\}$, in which $\mathbf{f}$ is the output corresponding to input $\mathbf{X}$, so the mean and variance functions of the output vector are given by

$$\boldsymbol{\mu}\left(\mathbf{X}^* | D\right) = K\left(\mathbf{X}^*, \mathbf{X}\right) K\left(\mathbf{X}, \mathbf{X}\right)^{-1} \mathbf{f} \tag{5}$$

$$\boldsymbol{\Sigma}\left(\mathbf{X}^* | D\right) = K\left(\mathbf{X}^*, \mathbf{X}^*\right) - K\left(\mathbf{X}^*, \mathbf{X}\right) K\left(\mathbf{X}, \mathbf{X}\right)^{-1} K\left(\mathbf{X}, \mathbf{X}^*\right) \tag{6}$$

$K(a,b)$ is the covariance function to describe the similarity of two variables a and b, both of which can be scalars, vectors or matrices. When both are scalars, it is written as k in Eq. (3). A common squared exponential covariance function is used in this example.

$$\mathrm{cov}\left(f\left(x^{(p)}, x^{(q)}\right)\right) = k\left(x^{(p)}, x^{(q)}\right) = a \cdot \exp\left(-\frac{l^2}{2}\left(x^{(p)} - x^{(q)}\right)^2\right) \tag{7}$$

The updating of Gaussian process is also computationally simple from this perspective. The posterior predictive distribution at least provides two pieces of information: (1) the expectation of the predicted responses regarding discretized inputs, and (2) the uncertainty or variance at each prediction. Recall from the previous introduction of “exploitation-exploration” tradeoff, and we are more interested at the area of low-prediction (for the local minimums of the fission product releases) and high-uncertainty (for the jump among local minimums).

Let us take a closer look at the Bayesian optimization with a simple example. The “black-box” objective function is plotted in Fig. 3 as the red curve, which is unable to know by us beforehand. The predictability of Gaussian processes is largely relied on the setting of an appropriate covariance function, and finally, it will affect the efficiency of the optimum finding. The squared exponential covariance function in Eq. (7) is used, and $a = 20$ and $l = 1$ are two hyper-parameters that are determined beforehand. The definition of the covariance applied can be explained in an easy-understanding way. The more similar two inputs look like, the more strong correlation two corresponding outputs will have. The mean of prediction function is plotted as the blue lines in Fig. 3, and the gray area is the predicted uncertainty, where the uncertainty is less near the observed data points. Therefore, the acquisition function, which describes our interests of next query, can be defined as Eq. (8), and we set $\tau = 5$ here. The labels of all axes in Fig. 3 are omitted since the example is used for illustration only.

$$a(x) = \tau \cdot \sigma(x) - \mu(x) \tag{8}$$

The plot of acquisition function $a(x)$ along the x-axis is drawn in the lower part of Fig. 3 as the blue contour, which guide us to find next possible minimum. The acquisition function shows the compromising between the mean and variance, and guides us to an area where minimum locates or, at appropriate timing, jump to unknown areas where other troughs locate. To begin with, we have no information about the objective function so that a random input has been chosen and then evaluated. The predictive function is simultaneously updated with the upcoming simulation data. Then, based on the result of the acquisition function of Eq. (8), the next interested point has been guided to the leftmost point of the x-axis, and the objective function is evaluated again. With more simulations are performed, the optimum is nearer and nearer to be found. As the results show, the global minimum is found at Round No.13. The efficiency and advantage of Bayesian optimization can be visualized.

IV. OPTIMIZATION ANALYSIS OF VENTING OPERATIONS AND RESULTS

When apply the foregoing approach to the severe accident mitigation analysis, the most reliable containment-venting strategy can be designed to protect the containment vessel through S/C vent system while restrain the release of fission products from the containment vessel. In Table 1, the four adjustable factors and one fixed factor are selected as the most important inputs for the venting operation. The complex problem is simplified as the optimization of a “black-box” function with four uncertain inputs. The general logics of venting as well as the setting of input space are provided in Table 2.

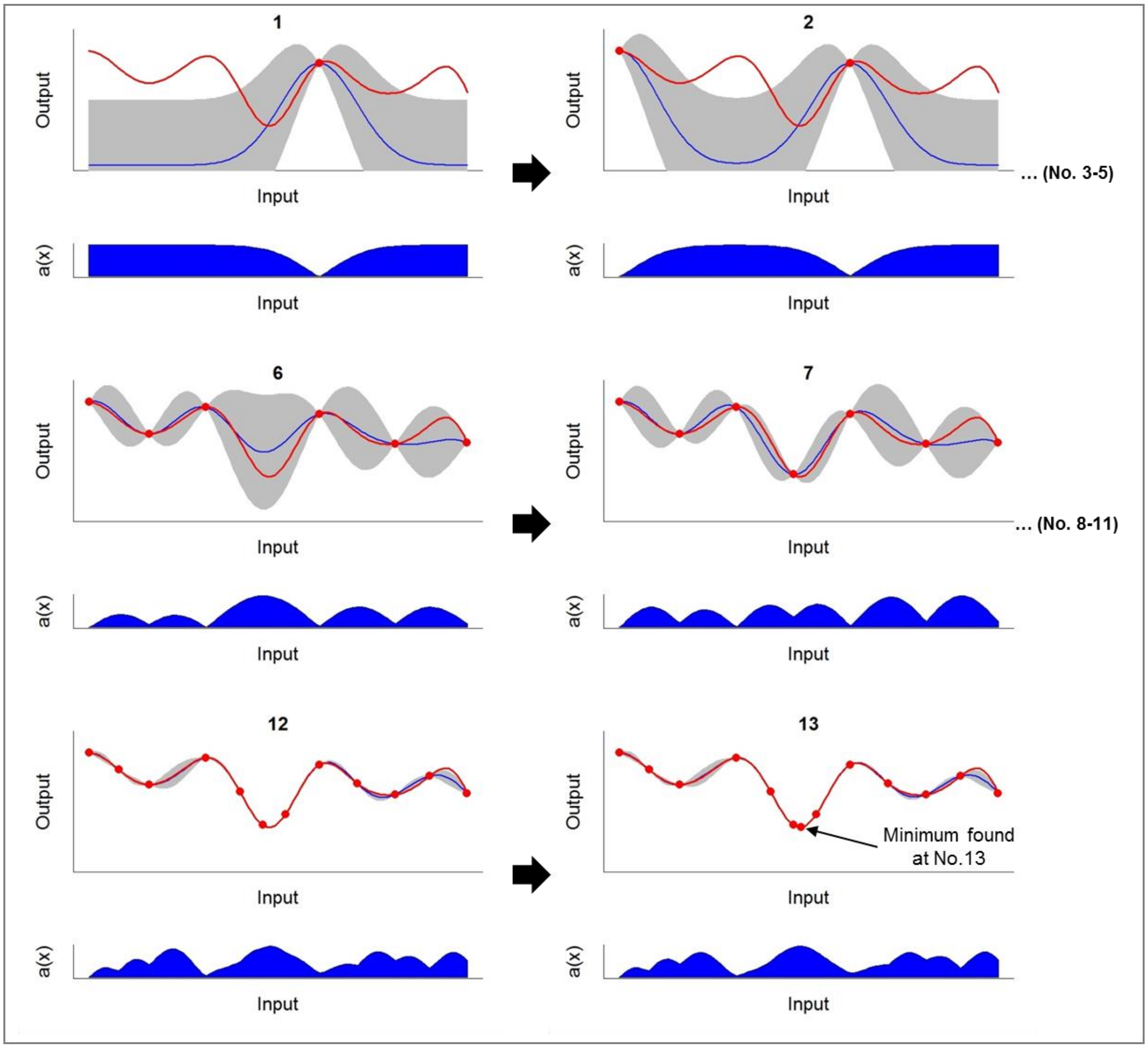

Fig. 3. The demonstration of 1-dimensional Bayesian optimization using a Gaussian process regression model (the objective function has no practical meaning and labels of axes are ommitted for easy-understanding)

Table 2. Logical rules of S/C venting

S/C Vent Criteria	Conditions	Range of Parameters
Forced open	$\text{Pressure}_{\text{D/W}} > x_1$	$x_1 \in \left(4.857\times10^5, 6.779\times10^5\right]$ Pa
Conditional open	$\left(\text{Pressure}_{\text{D/W}} > x_2\right) \cap \left(\text{Concentration}_{\text{FPs in D/W}} < x_3\right) \cap \left(\text{pH}_{\text{S/C Pool}} > x_4\right)$	$x_2 \in \left[4.857\times10^5, x_1\right]$ Pa; $x_3 \in [0, 0.05]$; $x_4 \in [5, 9]$
Forced Close	$\text{Pressure}_{\text{D/W}} < x_5$	$x_5 = 2.935\times10^5$ Pa

Three representative species of radionuclides considered in the paper include: iodine (I), cesium (Cs) and tellurium (Te). Chemical forms of them include: CsI, I_2, high- and low-volatile organic iodines, Cs_2MoO_4, and Te. It is noted that noble gases are not taken into account in the present analysis since their removal due to the deposition and scrubbing is not expected. The transportation of radionuclides within the containment, which are affected by many complex physical/chemical processes and thermal-hydraulic conditions, and venting operations will determine overall quantity of fission product release. The total initial core inventory of these representative species is 1401.781 moles. The severe accident simulation has been performed with the THALES2/KICHE code.

Some details of the surrogate model construction using Gaussian process are provided. Because there are magnitude discrepancies among four control parameters, for example, the order of pressure higher than that of in-containment radioactive concentration, the adjusted covariance function, instead of Eq.(7), for the Gaussian process model is constructed as follows.

$$\begin{aligned}\mathrm{cov}\left(f\left(\mathbf{x}^{(p)},\mathbf{x}^{(q)}\right)\right) &= K\left(\mathbf{x}^{(p)},\mathbf{x}^{(q)}\right)\\ &= \exp\left(-\frac{9}{2\times10^{10}}\left(x_1^{(p)}-x_1^{(q)}\right)^2-\frac{9}{2\times10^{10}}\left(x_2^{(p)}-x_2^{(q)}\right)^2-\frac{1}{2\times10^{-4}}\left(x_3^{(p)}-x_3^{(q)}\right)^2-\frac{1}{2}\left(x_4^{(p)}-x_4^{(q)}\right)^2\right)\end{aligned} \tag{9}$$

The posterior predictive distribution can be obtained based on Eq. (4). The modified acquisition function is defined based on predictive means and variances, similar to Eq. (8). The parameter of the acquisition function is adjusted, and τ is set to be 1, with a subjective judgment of the trend between exploration and exploitation.

$$a(\mathbf{x})=\sigma(\mathbf{x})-\mu(\mathbf{x}) \tag{10}$$

If we increase the pressure of venting activation, the risk of overpressure containment failure will increase; inversely, if the pressure is reduced, more fission products will be released through the venting system. In essence, the consideration of both containment failure and fission product release needs to be balanced, for the determination of a venting plan. As a preliminary research, however, we only consider the timing and conditions of the venting on the fission product release. We use the previously introduced Bayesian optimization to search the effective venting strategy, with a comparison with the pure random search by using the Monte Carlo method. First executions of both methods are randomly sampled from the input space. As demonstrated in Fig. 4, each output is distributed in a random way when the Monte Carlo random search is applied; on the contrary, the minimum (total release: 2.301 moles) is found by the Bayesian optimization method in a faster manner, the first one found at No.2, and a number of optical venting plans (5 times in a total of 14 code executions) with the same quantity of low-level releases are also found. Bayesian optimization shows advantage in efficiency to random search, by which one global minimum has been reached with the present investigation. The minimal release is less than that of early-venting example, but not significant.

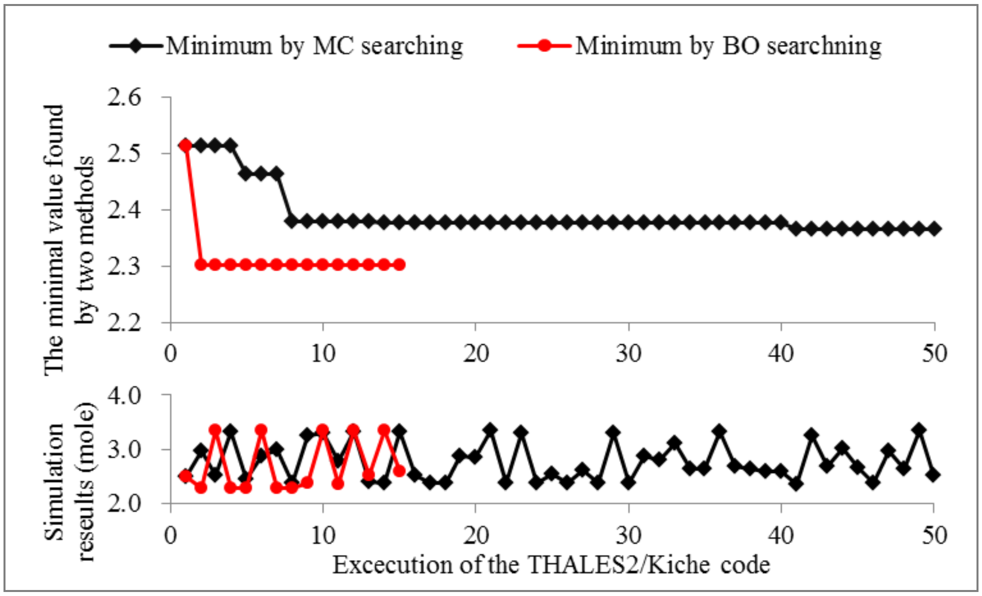

Fig. 4. Searching of the best S/C venting operation (The upper is the comparison between Monte Carlo Searching and Bayesian optimization search, by which is minimum is found at the second time of code execution, and the Bayesian optimization method shows advantages on efficiency; The lower is the record of all simulation results, and the Bayesian optimization found more alternative plans of the minimal fission product releases)

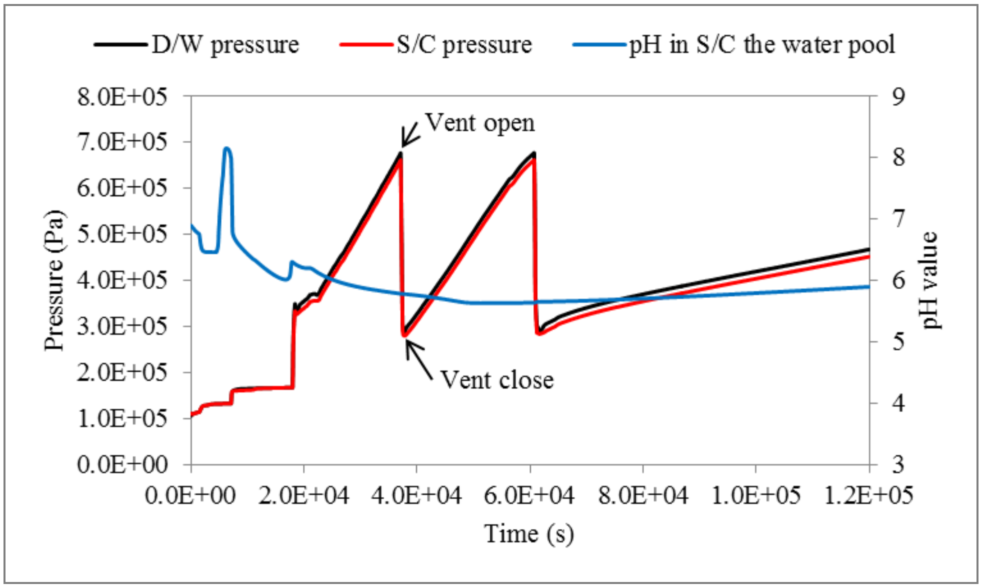

Fig. 5. Containment pressure and S/C pH change with time of the situation with the least fission product release of 2.301 moles (one of available prameter setting: $x_1 = 6.779\times10^5, x_2 = 4.857\times10^5, x_3 = 1.0\times10^{-4}, x_4 = 9.0$)

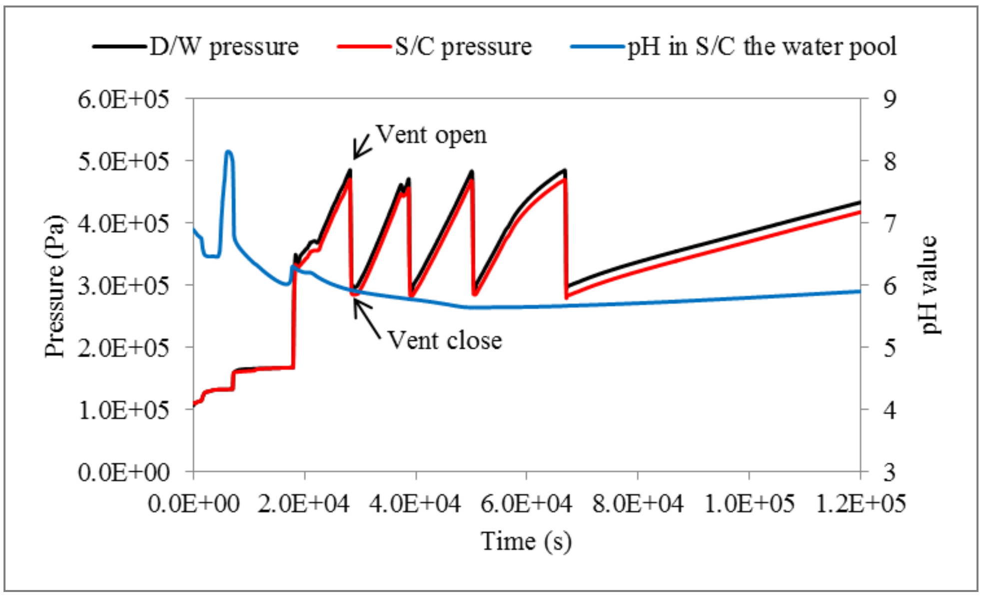

Fig. 6. Containment pressure and S/C pH change with time of a early-vent investigation with a release of 3.361 moles (the pventing parameter setting: $x_1 = 4.857\times10^5, x_2 = 4.857\times10^5, x_3 = 1.0\times10^{-4}, x_4 = 9.0$)

As an example of the strategies with least release, which is a case of delayed venting, the pressure changes in the D/W and S/C and pH value of the S/C water are provided in Fig. 5. Under the current conditions, the late-venting can provide more time for the reduction of airborne amount of fission products in D/W so that the fission product release can be mitigated. Since the overpressure failure probability of the containment vessel is not taken in account in the current paper, it can be foreseen that the setting of too high forced-open pressure would cause uncontrollable release of fission products so that the overall release might be high. According to the experimental and analytical researches of iodine chemistry in reactor cooling systems[19], the presence of gaseous molybdenum trioxide and molybdic acid in the cooling system has affected the iodine speciation, and Cs_2MoO_4 is treated as the main chemical form of Cs by inhibiting the formation of CsI. The existence of organic impurities, caused by the elution of organic solvents from the containment paints, results in the formation of organic iodine[9] in the current study.

As a demonstration of the effect of earlier-venting on the release of fission products, we also provide the results in Fig. 6, where the simulation results of containment pressures and pH value, with the progress of time, are given. Four times of S/C venting operate for depressurization of containment and the overall release of representative fission products from the containment vessel is 3.361 moles (the sum of representative fission products). Compared the result of Fig.5 and Fig.6, the delayed venting scenarios reduces the release of fission products. It can be foreseen that, as previously described, the risk of containment overpressure failure could become higher for the delayed venting. Further investigation on this point is considered to be necessary.

V. CONCLUSIONS

A Bayesian optimization approach has been proposed to efficiently search the optimal solutions of objective functions, and the crucial containment venting problem, under the condition of a BWR severe accident, is taken as an example of application. The Bayesian optimization methodology, when applied to practical nuclear reactor severe accident analysis, has been proven of several obvious advantages. The simulation-based analysis, of the containment venting operations, provides more sound evidence for the consequence mitigation, and also shows the improvement on efficiency compared with traditional Monte Carlo method. The conclusions are summarized as follows.

(1) Different venting operations, during a severe accident, are investigated through the simulation of the severe accident code, THALES2/KICHE. The responses of the reactor systems and overall fission product release are computed, and all of them combined can work as indices for the determination of a better venting plan. A number of venting strategies are identified as effective in controlling fission product release. Mainly, two types are found: first, depressurize the containment through S/C at the highest tolerable pressure; second, depressurize early when the contaminant level is low and the pH level in S/C satisfies certain source term assumption. The first plan is better than the second in the current study, but it also involves more risk of overpressure containment failure. Further investigation on venting optimization with consideration of containment overpressure failure is required.

(2) The surrogate model, constructed via Gaussian process, is nonparametric and flexible. It means that when more simulation data are obtained as the investigation goes on, the predictability of the surrogate model will improve accordingly. The complexity of the surrogate model is determined by the simulation results. This property enables the realization of the adaptive sampling scheme, which improves the optimum-searching efficiency.

(3) The methodology can be applied to wider analysis of nuclear reactor accidents, including Level 3 probabilistic risk assessment (PRA). When a problem gets more complex as more computational codes are coupled, the benefit of a surrogate model, as an aid, would be more outstanding.

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