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Original Article

# Bayesian Optimization Analysis of Containment-Venting Operation in a Boiling Water Reactor Severe Accident

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ABSTRACT

Containment venting is one of several essential measures to protect the integrity of the final barrier of a nuclear reactor during severe accidents, by which the uncontrollable release of fission products can be avoided. The authors seek to develop an optimization approach to venting operations, from a simulation-based perspective, using an integrated severe accident code, THALES2/KICHE. The effectiveness of the containment-venting strategies needs to be verified via numerical simulations based on various settings of the venting conditions. The number of iterations, however, needs to be controlled to avoid cumbersome computational burden of integrated codes. Bayesian optimization is an efficient global optimization approach. By using a Gaussian process regression, a surrogate model of the "black-box" code is constructed. It can be updated simultaneously whenever new simulation results are acquired. With predictions via the surrogate model, upcoming locations of the most probable optimum can be revealed. The sampling procedure is adaptive. Compared with the case of pure random searches, the number of code queries is largely reduced for the optimum finding. One typical severe accident scenario of a boiling water reactor is chosen as an example. The research demonstrates the applicability of the Bayesian optimization approach to the design and establishment of containment-venting strategies during severe accidents.



## 1. Introduction

The establishment of strategies in response to severe accident conditions is fraught with various 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 the final mitigation of radiological consequences. Because of the complexity of the overall situation, most decisions for severe accident management measures are

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currently made by expert judgement. 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, as is especially the case in many engineering fields, it is called a “black-box” objective function, such as an integral severe accident code for an experimental facility. The only way to obtain corresponding outputs of the “black-box” function is to evaluate it, and this usually requires computational/practical effort, which is sometimes so expensive as to be unaffordable. To overcome the inefficiency of random or grid searches for optimal solutions, we can adopt methods of deterministic global searching [2] or stochastic methods using Bayesian theory [3]. A simulation-based framework using the latter approach has been proposed; then, as a demonstration, a containment-venting operation under severe accident conditions in a boiling water reactor (BWR) 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 does not include 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. Under severe accident scenarios, venting of a containment vessel (involving the removal of steam, hydrogen, and other gases) might be required to prevent containment failure resulting from overpressure [4]. One primary requirement in Order EA-13-109 issued by the United States 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 release. 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, their effectiveness at ensuring containment protection and consequence mitigation needs to be inspected. To find the optimal setting of these influential factors with a minimization of fission-product release, queries via computer simulations using integrated severe accident codes are required.

The Japan Atomic Energy Agency has been developing the THALES2 code to analyze severe accident progression and estimate source terms for Level 2 probabilistic risk assessment [6]. In recent years an independent computer code for iodine chemistry simulation, KICHE [7,8], has been coupled with THALES2 through an interface program developed for the exchange of input/output between the two codes [9]. THALES2/KICHE is an integrated and fast-running severe accident code that 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 a consideration of iodine chemical reaction kinetics in aqueous phase, etc.

This 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 radioactive release from the containment vessel.

## 2. Severe accident analysis via THALES2/KICHE

A 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: reactor core, upper plenum, steam dome, downcomer, lower plenum, and recirculation loops A and B. The containment vessel model comprises the drywell (D/W), S/C, pedestal, and vent pipes that connect the D/W and S/C. The environment volume is connected to the reactor building and S/C, which represent the paths of containment leaks and the S/C vent.

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

As an example, one of several typical BWR severe accident sequences [11], TQUV (a transient (T) followed by failure of the feedwater system (Q), the high-pressure coolant injection system (U), and the low-pressure coolant injection system (V) with depressurization of reactor coolant system), is chosen to

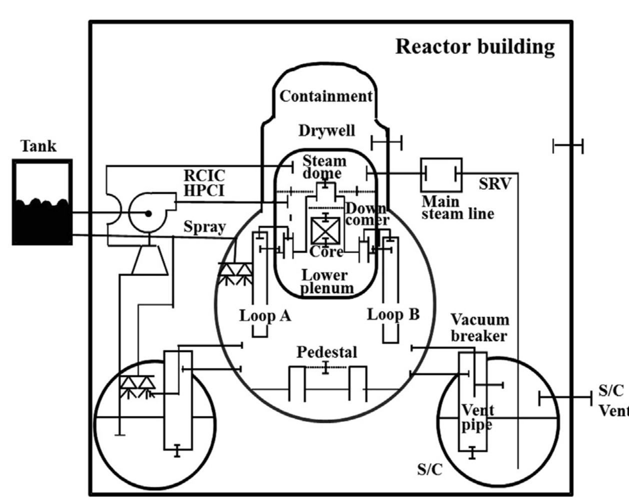


**Fig. 1 – Control volume nodalization for THALES2/KICHE modeling. HPCI, high pressure coolant injection system; RCIC, reactor core isolation cooling system; S/C, suppression chamber; SRV, safety relief valve.**

demonstrate the current approach of global optimization. Immediately after the occurrence of the transient, the reactor is scrammed and successfully depressurized. Upon 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 relief valves 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 the 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 the containment is to minimize airborne amounts in the containment, including the D/W and S/C, during venting [1]. From the point of view of 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 radioactive material release, although no corresponding measurement is currently made for this value. Important factors also include the opening and closing pressures for the 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 release from the containment. The definition and notation of each factor are summarized in Table 1.

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

## 3. Bayesian optimization with a Gaussian process regression model

The problem of finding a reliable venting strategy, which is a strategy to control the release of fission products at a minimal level, can be converted to the minimizing of an unknown or "black-box" function:

$$\mathbf{x}^* = \arg\min_{x \in X} f(\mathbf{x}) \tag{1}$$

Here, $f(\cdot)$ is the objective function with respect to the controlling inputs $x \in X$, and $x^*$ is the specific input we try to find which will minimize the response of the objective function $f(\cdot)$. In severe accident analysis, the objective function $f(\cdot)$ can be equivalently treated using computer codes THALES2/KICHE, and hence we need to query the function value at arbitrary $x \in X$ through an execution of the code.

**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 |

D/W, drywell; S/C, suppression chamber.

The optimization algorithm should quickly find local optimums while easily jumping out to other areas to find the next local/global optimum; this process is called the tradeoff of "exploitation" and "exploration". The "exploitation" promotes search in an area of "more interests" where local optimums are located; the "exploration" promotes search in an area of "more potential values". A more detailed introduction to Bayesian optimization can be found in the references [12–14]. In this paper we provide an introduction from the perspective of a surrogate model [15,16]. The objective function is unknown within the Bayesian framework, therefore, the main tactic is to treat the function as a random one, which we name 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 with useful information for the prediction of the 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 schemes of Bayesian optimization. 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 the Gaussian process regression model). We name the method an "adaptive sampling method" because the choice of input is guided by the surrogate model.

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

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

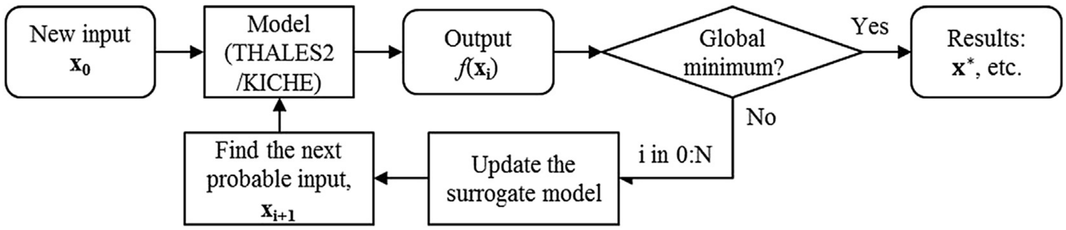


**Fig. 2 – Adaptive-sampling procedure of Bayesian optimization.**

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

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

Here, $GP$ is the Gaussian process. The Bayesian update of Eq. (2) converts to an update of the mean function $m(x)$, and the covariance function $k(x, x')$, both of which are written in 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.

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

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

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

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

$K(a, b)$ is the covariance function used to describe the similarity of two variables $a$ and $b$, both of which can be scalars, vectors, or matrices. When both are scalars, the covariance function is written as $k$ in Eq. (3). A common squared exponential covariance function is used in this example. The covariance function specifies the covariance between pairs of two random outputs, which can be written as a function of two inputs ($x^{(p)}$ and $x^{(q)}$). The covariance is almost unity then two corresponding inputs are very close, and decrease as their distance in the input space increases.

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

From this perspective, the updating of the Gaussian process is also computationally simple. The posterior predictive distribution provides at least two pieces of information: (1) the expectation of the predicted responses regarding discretized inputs; and (2) the uncertainty or variance of each prediction. It was seen in the previous introduction of the "exploitation–exploration" tradeoff that we are more interested in 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 a red curve, indicating what is not possible for us to know beforehand. The predictability of the Gaussian processes largely relies on the setting of an appropriate covariance function; finally, this function will affect the efficiency of the optimum finding. The squared exponential covariance function in Eq. (7) is used, $a = 20$ and $l = 1$ are two hyperparameters that are determined beforehand. The definition of the covariance applied can be explained in an easy-to-understand way. The more similar two inputs look, the stronger the correlation will be between the two corresponding outputs. The mean of the prediction function is plotted as the blue lines in Fig. 3; the gray area is the predicted uncertainty, in which the uncertainty is lower near the observed data points. Therefore, the acquisition function, which can help to find next query of interest, 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 the acquisition function $a(x)$ along the x-axis is drawn in the lower part of Fig. 3 as a blue contour, which guides us to find the next possible minimum. The acquisition function shows a compromise between the mean and the variance, and guides us to an area where the minimum is located or, at appropriate timing, jumps to unknown areas where other troughs are located. To begin with we have no information about the objective function, so a random input has been chosen and then evaluated. The predictive function is simultaneously updated with the upcoming simulation data. Then, based on the results of the acquisition function of Eq. (8), the next point of interest has been set as guided to the leftmost point of the x-axis, and the objective function is evaluated again. When more simulations are performed the

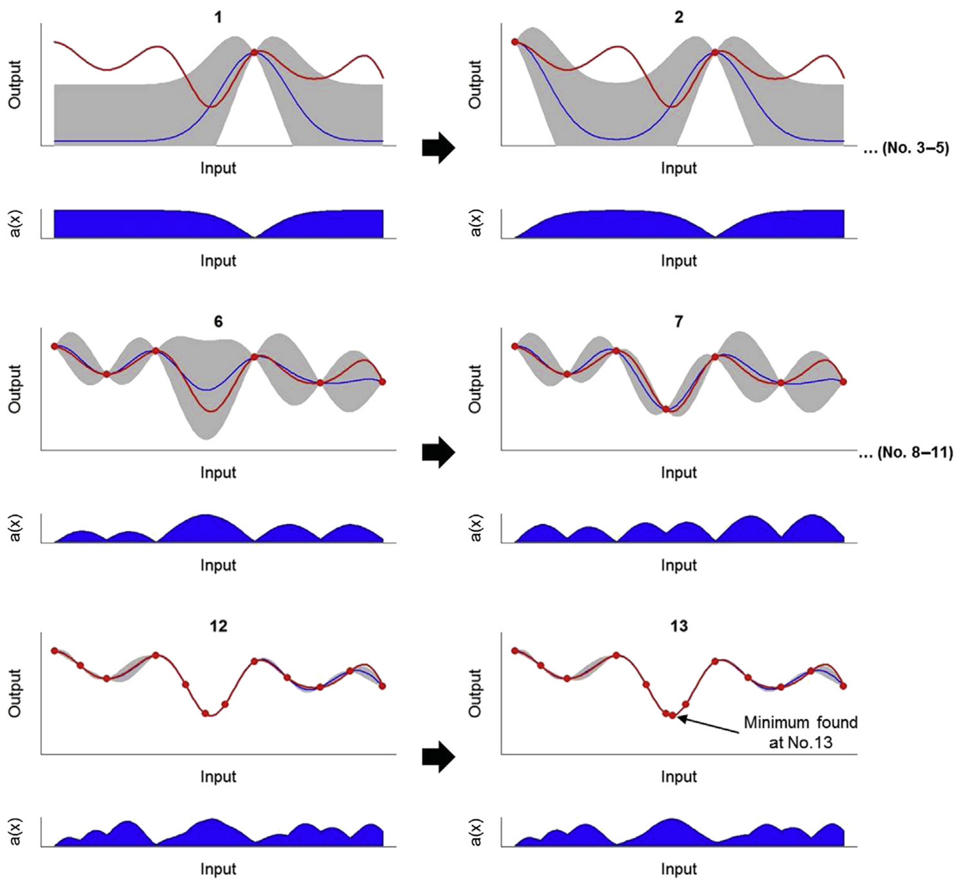


**Fig. 3 – Demonstration of one-dimensional Bayesian optimization using a Gaussian process regression model (the objective function has no practical meaning and labels of axes are omitted for easier understanding).**

optimum is closer and closer to being found. As the results show, the global minimum is found in Round No. 13. This helps us to visualize the efficiency and advantage of Bayesian optimization.

## 4. Optimization analysis of venting operations and results

By applying the foregoing approach to severe accident mitigation analysis, the most reliable containment-venting strategy can be designed to protect the containment vessel through the S/C vent system, while restraining 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 logic of venting, as well as the setting of the input space, are shown in Table 2.

Three representative species of radionuclides considered in the paper include: iodine (I), cesium (Cs), and tellurium (Te). Chemical forms of these include: CsI, $I_2$, high- and low-volatile organic iodines, $Cs_2MoO_4$, and Te. It should be noted that noble gases are not taken into account in the present analysis because their removal via deposition and scrubbing is not expected. The transportation of radionuclides within the containment (which is affected by many complex physical/chemical processes and thermal–hydraulic conditions) and the venting operations will determine the overall quantity of fission product-release. The total initial core inventory of these representative species is 1,401.781 mol. The severe

**Table 2 – Logical rules of suppression chamber venting.**

| S/C vent criteria | Conditions | Range of parameters |
|---|---|---|
| Forced open | $Pressure_{D/W} > x_1$ | $x_1 \in (4.857 \times 10^5, 6.779 \times 10^5]$ Pa |
| Conditional open | $(Pressure_{D/W} > x_2) \cap (Concentration_{FPs\ in\ D/W} < x_3) \cap (pH_{S/C\ Pool} > x_4)$ | $x_2 \in [4.857 \times 10^5,\ x_1]$ Pa; $x_3 \in [0,\ 0.05]$; $x_4 \in [5,\ 9]$ |
| Forced close | $Pressure_{D/W} < x_5$ | $x_5 = 2.935 \times 10^5$ Pa |

D/W, drywell; S/C, suppression chamber.

accident simulation has been performed with the THALES2/KICHE code.

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

$$\mathrm{cov}\left(f\left(\mathbf{x}^{(p)},\mathbf{x}^{(q)}\right)\right) = K\left(\mathbf{x}^{(p)},\mathbf{x}^{(q)}\right)$$
$$= \exp\left(-\frac{9}{2\times 10^{10}}\left(x_1^{(p)}-x_1^{(q)}\right)^2 - \frac{9}{2\times 10^{10}}\left(x_2^{(p)}-x_2^{(q)}\right)^2 - \frac{1}{2\times 10^{-4}}\left(x_3^{(p)}-x_3^{(q)}\right)^2 - \frac{1}{2}\left(x_4^{(p)}-x_4^{(q)}\right)^2\right) \quad (9)$$

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 $\tau$ is set at 1, providing a subjective judgment of the trend between exploration and exploitation.

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

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, considerations of both containment failure and fission-product release need to be balanced for the determination of a venting plan. As this is only preliminary research, however, we consider only the effects of the timing and conditions of the venting on the fission-product release. We use the previously introduced Bayesian optimization to search for an effective venting strategy, with a comparison with a purely random search using the Monte Carlo method. First executions of both methods are randomly sampled from the input space. As can be seen in Fig. 4, each output is distributed in a random way when the Monte Carlo random search is applied; conversely, the minimum (total release: 2.301 mol) can be found by using the Bayesian optimization method, and in a faster manner, with the first minimum found at No. 2; a number of optical venting plans (five times in a total of 14 code executions) with the same quantity of low-level release are also found. Bayesian optimization shows advantages in efficiency compared with a random search, in which only one global minimum has been reached in the present investigation. The minimal release is less than that of the early-venting example, but not significant.

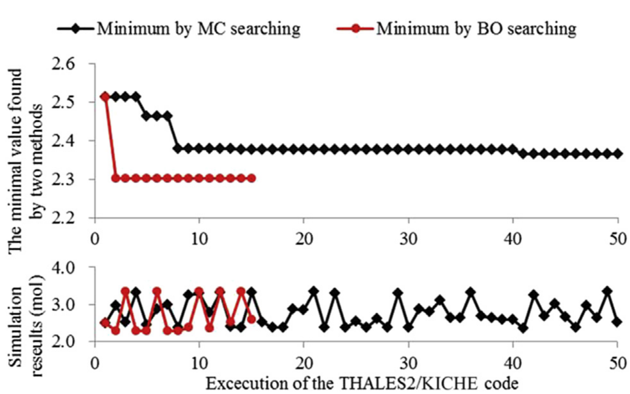


**Fig. 4 – Searching for the best S/C venting operation. (The upper is the comparison between Monte Carlo searching and Bayesian optimization search, by which the minimum is found at the second time of code execution; the Bayesian optimization method shows advantages in terms of efficiency. The lower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

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 the pH value of the S/C water are provided in Fig. 5. Under the current conditions, late venting can provide more time for the reduction of the airborne quantity of fission products in the D/W, so that fission-product release can be mitigated. Since the overpressure failure probability of the containment vessel is not taken into account in the current paper, it can be foreseen that the setting of a too high forced-open pressure would cause uncontrollable release of fission products, such that the overall release might be high. According to experimental and analytical research into iodine chemistry in reactor cooling systems [19], the presence of gaseous molybdenum trioxide and molybdic acid in the cooling system can affect 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

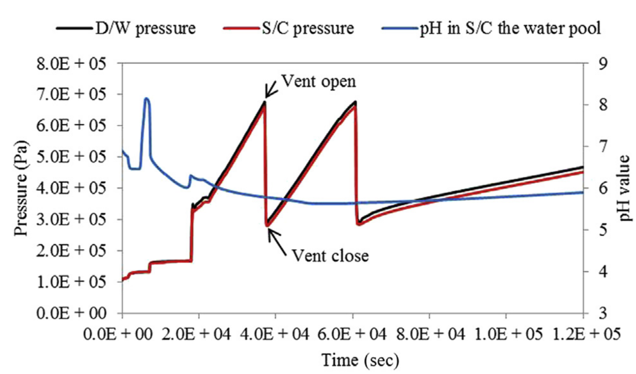


**Fig. 5 – Containment pressure and S/C pH change with time of the situation with the least fission-product release of 2.301 mol (one of available parameter settings: $x_1 = 6.779 \times 10^5, x_2 = 4.857 \times 10^5, x_3 = 1.0 \times 10^{-4}, x_4 = 9.0$). D/W, drywell; S/C, suppression chamber.**

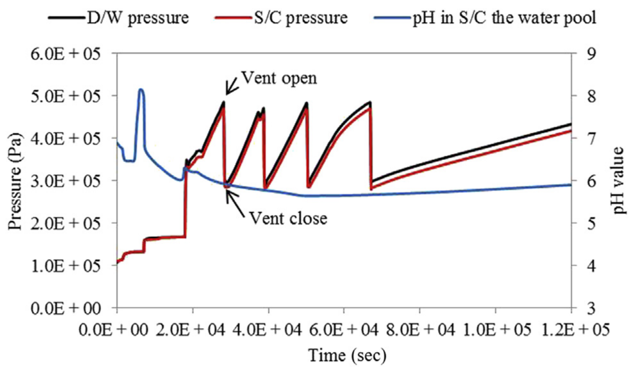


**Fig. 6 – Containment pressure and S/C pH change with time of early-vent investigation with a release of 3.361 mol (the venting parameter setting: $x_1 = 4.857 \times 10^5, x_2 = 4.857 \times 10^5, x_3 = 1.0 \times 10^{-4}, x_4 = 9.0$). D/W, drywell; S/C, suppression chamber.**

by the elution of organic solvents from containment paints, was found to result 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 results in Fig. 6, in which the simulation results of the containment pressures and pH value, with the progress of time, are given. Four times venting of the S/C led to the depressurization of the containment; the overall release of representative fission products from the containment vessel is 3.361 mol (the sum of the representative fission products). Comparing the results shown in Fig. 5 and Fig. 6, the delayed venting scenarios reduce the release of fission products. It can be foreseen that, as previously described, the risk of containment overpressure failure could become higher during delayed venting. Further investigation of this point is considered to be necessary.

## 5. Conclusion

A Bayesian optimization approach has been proposed to efficiently search for optimal solutions of the objective functions; a crucial containment-venting problem under the condition of a BWR severe accident is provided as an example of application. The Bayesian optimization methodology, when applied to practical nuclear reactor severe accident analysis, has been proven to have several obvious advantages. The simulation-based analysis of the containment-venting operations provides more sound evidence of consequence mitigation, and also shows improvement of the efficiency compared with the traditional Monte Carlo method. The conclusions can be 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 the overall fission-product release are computed; all of these factors 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, to depressurize the containment through the S/C at the highest tolerable pressure; second, to depressurize early when the contaminant level is low and the pH level in the S/C satisfies a 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 of venting optimization with a consideration of the containment overpressure failure is required.

(2) The surrogate model, constructed via a Gaussian process, is nonparametric and flexible. This 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 an adaptive sampling scheme, which improves the optimum searching efficiency.

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

## Conflicts of interest

All authors have no conflicts of interest to declare.


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