# Surrogate Model for Recirculation Phase LBLOCA and DET Application

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## 1. Introduction

Code surrogates are mathematical models that approximate the input/output relationship of more complex computer code simulations. Surrogates, also called response surfaces, metamodels, and code emulators, are fast running making them attractive to applications such as design optimization and uncertainty quantification where many simulations need to be performed and direct use of the computer code is computationally prohibitive. In the nuclear safety field, response surfaces were used in the first demonstration of the code scaling, applicability, and uncertainty (CSAU) methodology to quantify the uncertainty of the peak clad temperature (PCT) during a large-break lossof-coolant accident (LBLOCA). Surrogates could have applications in other nuclear safety areas such as dynamic probabilistic safety assessment (PSA). Dynamic PSA attempts to couple the probabilistic nature of failure events, component transitions, and human reliability to deterministic calculations of timedependent nuclear power plant (NPP) responses usually through the use of thermal-hydraulic (TH) system codes. The overall mathematical complexity of the dynamic PSA architectures with many embedded computational expensive TH code calculations with large input/output data streams have limited realistic studies of NPPs.

This paper presents a time-dependent surrogate model for the recirculation phase of a hot leg LBLOCA in the OPR-1000. The surrogate model is developed through the ACE algorithm [1], a powerful nonparametric regression technique, trained on RELAP5 simulations of the LBLOCA. Benchmarking of the surrogate is presented and an application to a simplified dynamic event tree (DET).

#### 2. Modeling Recirculation Phase of LBLOCA

## 2.1. OPR-1000 systems description

An LBLOCA is postulated to occur in the hot leg of the OPR-1000, a two-loop pressurized water reactor (PWR) with a rated power of 2815 MWt. The reactor coolant system (RCS) consists of the core, 4 cold legs, 2 hot legs, 2 steam generators, and pressurizer. The safety injection (SI) systems replenish the RCS inventory following a LOCA and ensure long term cooling of the core. The high pressure safety injection (HPSI) system, low pressure safety injection (LPSI) system, and safety injection tanks (SIT) interface with the RCS at the SI headers on the cold leg piping. The HPSI and LPSI systems each have two pumps with design flows of 815 gpm and 4200 gpm, respectively. The containment spray (CS) system suppresses containment pressure and temperature and removes heat to the ultimate heat sink. The containment spray (CS) system consists of two pumps with design flows of 3890 gpm, shutdown cooling heat exchangers, and spray headers.

## 2.2. TH behavior during LBLOCA

Following the initial blowdown and reflood, the LBLOCA can be divided into 3 major phases for the long term cooling of the core: injection phase, recirculation phase, and simultaneous hot and cold leg injection. During the injection phase, all HPSI, LPSI, and CS pumps in their initial configuration draw suction from the refueling water storage tank (RWST). When the RWST inventory is depleted, the recirculation actuation signal (RAS) is sent and the LPSI pumps are automatically tripped. The HPSI and CS pump suction are automatically switched to the containment sumps where spilled water from the break and condensed steam and CS water collects. Operators must manually isolate the RWST and verify that sufficient sump conditions exist for recirculation. The sump water temperature can be much higher than the RWST water temperature and is a function of the total energy released from the RCS through the break flow and the operation of the CS system integrated over the transient time. At some time after recirculation begins, operators must manually realign some of the HPSI pump discharge to the hot legs for simultaneous hot and cold leg injection to ensure a sufficient flushing flow exists across the core to prevent boron precipitation.

The combined flow rate of the HPSI and LPSI pumps injecting large volumes of cold water from RWST to the RCS results in the single-phase flow and subcooling of the core during the injection phase. The RAS can be received as early as 20 minutes after a LBLOCA occurs when the decay power in the core is relatively high. The combination of high decay power, reduced SI flow rate after trip of LPSI pumps, and SI water from the sump that is closer to saturation conditions cause a rapid transition into two-phase flow in the top of the core increasing core boil-off and dropping the water level at the onset of recirculation. Subcooling of the core is gradually restored through decreasing decay power with time and continued recirculation through the HPSI and CS systems. This study investigates the time-dependent behavior of the core subcooling subject to uncertainties of the containment sump conditions and HPSI pump performance degradations. A surrogate model is constructed to predict the fraction of core subcooling.

Additionally, during the injection phase and early on in recirculation, reflux heat transfer conditions can exist in the steam generator (SG) of the intact loop. Because the RCS rapidly depressurizes during the blowdown and most of the RCS inventory is replaced with cold SI water, the primary side pressure and temperature can be lower than the large inventory of water in the shell side of the SG. Reflux heat transfer superheats residual steam and water on the tube side which can circulate through the cold leg piping mixing with SI water. Although the mass flow rates in the intact loop are small, the mixing can raise the enthalpy of the SI water reaching the core.

### 2.3. RELAP5 model

A RELAP5/MOD3.3 model of the Ulchin Units 3&4 NPP (UCN3&4), a reference OPR-1000, was used to simulate the LBLOCA and recirculation phase. The model is comprised of 250 hydrodynamic volumes, 280 hydrodynamic junctions and 259 heat structure representing all of the major components of the RCS. The RCS nodalization is shown in Fig. 1.

The HPSI and LPSI systems are modeled as timedependent volumes and junctions representing user defined time and system state dependent boundary conditions to the model. The pumps are modeled as junctions actuated by trip logic. Flow rate curves for the pumps are input as table lookup functions of pressure in the discharge legs of the cold leg piping. A degradation factor is applied to the HPSI pump curve to adjust flow rates. Time-dependent volumes representing the SI water source from the RWST or containment sumps define the temperature water flowing through the junctions.

RELAP5 is usually not used for containment analysis so the containment volumes and CS system are not explicitly modeled. The hot leg break is connected to time-dependent volumes representing the containment compartments providing sinks for water and steam that exit the break. A time-dependent pressure curve characteristic of a containment response to LBLOCA is input for the containment volumes.



Fig. 1. Nodalization for RELAP5 UCN3&4 model.

## 2.3. RELAP5 simulations

The RELAP5 UCN3&4 model was used to simulate 13 sequences of the recirculation phase of the hot leg LBLOCA. First, the injection phase of the LBLOCA was simulated assuming all HPSI, LPSI, and CS pumps operate at design capacities and the RAS time was calculated to occur at 1680 s assuming a 7.5% level setpoint for the RWST. The simulation was restarted for each of the 13 recirculation phase sequences with the assumed flow rate of the HPSI pumps and sump water temperature listed in Table I. HPSI flow rates were varied from 100% to 25% to represent a spectrum of possible degraded HPSI operation including 1 failed pump and decreased net positive suction head (NPSH). The sump water temperatures were varied from 300 K, the temperature of the RWST water during the injection phase, and 370 K which is close to saturation temperature of the RCS during recirculation. For sequences 12 and 13, the sump water temperature followed the ramp curve depicted in Fig. 2 where the temperature is assumed to linearly increase to saturation from the RAS time to 10,000 s and linearly decrease to 325 K at 20,000 s.

Table I. Design matrix of HPSI flow rate and containment sump temperature for RELAP5 recirculation phase simulations

r r						
Seq. #	HPSI Flow Rate Sump Temperature (I					
1	100%	300				
2	100%	325				
3	100%	350				
4	75%	300				
5	75%	325				
6	75%	350				
7	75%	370				
8	50%	300				
9	50%	325				
10	50%	350				
11	25%	300				
12	100%	Ramp				
13	50%	Ramp				



Fig. 2. Containment sump temperature curve for ramp cases in design matrix.

The results from the RELAP5 simulations of the recirculation phase are shown in Fig. 3. The plots of the subcooled water level V, the fraction of the core volume where single-phase flow and subcooling TH conditions exist, are normalized to the height of the top of the active fuel in the core. Figure 3 shows the rapid transition to two-phase flow in the core following RAS and the trip of the LPSI pumps and the gradual recovery of the subcooled water level with time. The transient behavior appears to be sensitive to both the HPSI flow rate and sump water temperature.



Fig. 3. Subcooled water level during recirculation.

## 3. Surrogate Model for Recirculation Phase

The computation time for each RELAP5 simulation presented in previous section is on the order of hours. In the context of PSA, there are several systems and subsystems and associated components whose successful operation, failures, and degradations determine the HPSI flow rate and sump water temperature that are the time-dependent boundary conditions to the UCN3&4 model. A dynamic PSA study may require many simulations to resolve the plant behavior subject to the performance of these

components and systems. In this section, we construct a surrogate model capable of predicting the subcooled water level in the core during the recirculation phase. The surrogate structure is proposed as a discrete time dynamic model and the functional form of the model is learned by performing regression on the RELAP5 simulations through the ACE algorithm.

### 3.1. Alternating conditional expectation algorithm

The ACE algorithm is a generalized nonparametric method that yields an optimal relationship between the dependent variable *y* and multiple independent variables  $\{x_{i}, i=1,...,p\}$  by obtaining one-dimensional transformations  $\theta(y)$  and  $\phi_{i}(x_{i})$  of each variable through an iterative procedure that maximizes the statistical correlation between  $\theta(y)$  and  $\sum_{i=1}^{p} \phi_{i}(x_{i})$ . A full derivation and algorithmic details can be found in Ref. [1]. The ACE algorithm procedure applied to a multivariate data set  $(X,y) = \{x_{ij}, y_{j}, i=1,...,p, j=1,...,n\}$  is given in Table II.



The key feature of the ACE algorithm is the localized smoothing operation S[.] in steps 2 and 3. The smoothing operation is the conditional expectation from which the name of the ACE algorithm is derived. The smoothing operation is

$$S[Z_k|z_j] = \sum_{k=j-M}^{j+M} W_k Z_k , \qquad (1)$$

a weighted average about a window of data points around point  $z_j$ . Each data smooth is a form of locally weighted regression. The weights  $W_k$  and window width 2M are determined by the type of smoothing operation which must be chosen by the user. This study used the 'acepack' package available in the R statistical program using the supersmoother [2], which adaptively varies the window width due to the local data characteristics. The ACE algorithm yields the nonlinear relationship through the transformations

$$\theta(y) = \sum_{i=1}^{p} \phi_i(x_i) + v .$$
<sup>(2)</sup>

The final nonlinear mapping from the inputs to the output variable involves taking the inverse transform

$$y = \theta^{-1} \left( \sum_{i=1}^{p} \phi_i(x_i) \right). \tag{3}$$

The model uncertainty v of the ACE surrogate can be estimated by calculating the weighted variance of  $\theta(y)$ using the converged transformed data points  $\theta(y_j)$  from the last iteration of the ACE algorithm [3]. The weighted variance using Eq. (1) is

$$s^{2}[Z_{k}|z_{j}] = \frac{\sum_{k=j-M}^{j+M} W_{k}(z_{k}-S[z_{k}|z_{j}])^{2}}{\frac{2M-1}{2M}\sum_{k=j-M}^{j+M} W_{k}} .$$
 (4)

#### 3.2. ACE surrogate for recirculation phase

In typical applications, surrogates are usually static input-output nonlinear mappings that predict limiting values of the output variable, such as PCT, without computing a complete time-dependent history of the system behavior. However, in dynamic PSA applications, the system state evolution under different operation conditions coupled to interactions with component transitions and human operator actions that can lead to safe or unsafe plant states is the desired result. Obtaining the system state evolution trajectories requires that complete simulations be performed. A dynamic code surrogate that can predict time-dependent system behavior will significantly reduce the computational burden compared to direct calculations with a TH code.

We propose the surrogate to take the general structure of a discrete time dynamic model

$$x(t_{k+1}) = F[x(t_k), \boldsymbol{u}(t_k), \boldsymbol{v}(t_k), \Delta t], \quad (5)$$

where system state *x* is advanced over discrete time steps {  $\Delta t = t_{k+1} - t_k$ } to predict the future state  $x(t_{k+1})$ from the previous state estimate  $x(t_k)$  and the input parameter vector *u* subject to model noise or uncertainty *v*. *F*[.] is possibly a nonlinear function. The system state is recursively calculated from  $t_0 \rightarrow t_N$ by setting  $x(t_{k+1}) \rightarrow x(t_k)$  after each evaluation of Eq. (5). The discrete time dynamic model implicitly treats the absolute transient time  $t_k$  as input parameters, which may be time-dependent functions.

For the recirculation phase surrogate, the system state variable is the subcooled water level V(t). The input parameters are sources of mass and energy flux into the RCS that drive the TH behavior. Four input

variables are decay power  $q_d(t)$ , subcooling enthalpy flow rate of the HPSI system  $h_p w_p$ , mass flow rate of HPSI system  $w_p$ , and ratio of subcooling enthalpy flow rate to decay power  $h_p w_p / q_d(t)$  which is a dimensionless number similar to the Stanton number. Equation (5) becomes

$$V_{k+1} = F\left[V_k, q_d, h_p w_p, w_p, \frac{h_p w_p}{q_d}, v_k, \Delta t\right].$$
 (6)

The purpose of the ACE algorithm is to the learn the functional form of F[.] from data of the 13 RELAP5 simulations. The decay power curve is available from the RELAP5 output and is the same for all sequences. The subcooling enthalpy flow rate of the HPSI system is defined as  $h_p w_p = (h_{sat} - h_{sump}) w_p$  where  $h_{sat}$  is the saturation enthalpy of the fluid in the RCS and  $h_{sump}$  is the enthalpy of the water in the containment sumps which is directly determined by the assumed temperature of the sump water during recirculation. The subcooling enthalpy flow rate represents the amount energy per unit time the liquid SI water can absorb without reaching saturation and generating steam. The mass flow rate of the HPSI system is also directly determined by the assumed flow rate used for each sequence.

For each sequence,  $V_{n+1}$  and  $V_n$  were extracted at  $\Delta t = 20$  s time steps from the RELAP5 output observing V does not change by more than a few percent in the data for this time scale. Combined with the decay power data and assumed HPSI flow rates and sump temperatures, the 13 RELAP5 sequences provide 15916 data points representing realizations of Eq. (5). Figure 4 shows the scatterplots of  $V_{n+1}$  as a function of each input variable. Visual examination of the scatterplots reveal very little information about the functional form of Eq. (6) except the strong linear correlation between  $V_{n+1}$  and  $V_n$  which is expected from the recursive relationship of the discrete time dynamic model structure.

Applying the ACE algorithm to the data sets yields the transformations shown in Fig. 5. The transformations provide smooth one-dimensional function forms for each variable and Eq. (6) is explicitly written as

$$\theta(V_{n+1}) = \phi_1(q_d) + \phi_2(h_p w_p) + \phi_3(w_p) + \phi_4\left(\frac{h_p w_p}{q_d}\right) + \phi_5(V_n) + v$$
$$V_{n+1} = \theta^{-1} \left(\phi_5(V_n) + \sum_{j=1}^4 \phi_j(x_j) + v\right).$$
(7)

One strength of the ACE algorithm as a nonparametric regression technique is that no *a priori* assumptions had to be made about the functional forms of the transformations in Fig. (5). The transformations were automatically learned by the ACE algorithm from the noisy RELAP5 data shown in Fig. (4).

Table III lists the ranges of the independent variable transformations and comparison to the range of  $\theta(V_{n+1})$ 

in the transform space as a measure of sensitivity or the importance of each variable. The range of the recursive component  $\phi_5(V_n)$  of the surrogate is equal to 73% of  $\theta(V_{n+1})$  followed by subcooling enthalpy flow  $\phi_2(h_pw_p)$ and decay power  $\phi_1(q_d)$  at 33% and 23%, respectively. The consequence of the discrete time dynamic system model structure is the direct correlation between  $V_{n+1}$ and  $V_n$  evident through the transformations  $\phi_5(V_n)$  and  $\theta(V_{n+1})$  which are nearly linear. The time step limits the deviation of  $V_{n+1}$  from  $V_n$  within a few percent so  $V_n$ must be the most important parameter that determines  $V_{n+1}$ . The other variables determine whether the water level increases or decreases from  $V_n$ .



Fig. 4. Scatterplots of subcooled water level *V* vs. input variables for ACE surrogate.

Table III. Range and sensitivity of ACE transformations

	min	max	$\Delta \phi$	% of $\theta$
$\theta$	-1.91	2.08	3.99	100
$\phi_1$	-0.39	0.54	0.93	23
$\phi_2$	-0.74	0.58	1.32	33
$\phi_3$	-0.06	0.04	0.10	3
$\phi_4$	-0.11	0.42	0.53	13
<u> ሰ</u> -	-1.43	1.47	2.90	73



Fig. 5. ACE transformations of smoothed RELAP5 data for subcooled water level surrogate.

Figure 6 shows the estimated variance of  $\theta(V_{n+1})$  calculated through Eq. (4). When the surrogate is used to predict  $V_{n+1}$  with Eq. (7),  $\nu$  represented by the variance of  $\theta(V_{n+1})$  must be propagated through the inverse transform  $\theta^{-1}(.)$  to obtain an uncertainty for  $V_{n+1}$ . Assuming the errors are normally distributed, a standard deviation of +/-0.05 is a good approximation of the uncertainty of  $V_{n+1}$ .



Fig. 6. Variance estimate of  $\theta(V_{n+1})$ .

## 3.3. Benchmarking surrogate vs. RELAP5 results

To test the predictive accuracy of the surrogate, the RELAP5 sequences in the training set are simulated with the ACE surrogate. RELAP5 sequences and the ACE predictions are compared in Fig. 7. The standard deviations presented with the ACE results represent the uncertainty of the ACE predictions. Two additional RELAP5 simulations were performed, Sequence 14 and Sequence 15, comprising a test set for cross-validation. Sequence 14 assumed 100% HPSI flow rate and a constant sump temperature of 335 K. Sequence 15 assumed 100% HPSI flow rate and a time-dependent

sump temperature curve shown in Fig. 8 obtained from the UCN3&4 FSAR [4].



Fig. 7. Comparison of RELAP5 simulations and ACE surrogate model estimates for recirculation phase.



Fig. 8. Containment sump temperature curve for Sequence 15.

The surrogate simulations were initiated at a transient time of 1680 s, the time of the RAS, and subcooled water level  $V_0 = 1$ . Using 20 s time steps, Eq. (7) was evaluated to obtain  $V_{n+1}$ . The ACE model uncertainty v discussed in Section 3 introduces uncertainty into each prediction  $V_{n+1}$ . From the recursive relationship  $V_{n+1} \rightarrow$  $V_n$ , the state estimate  $V_n$  becomes an uncertain input parameter to the surrogate, first undergoing the nonlinear transformation  $\phi_5(.)$  and subsequent transformation  $\theta^{-1}(.)$  after being combined with the model uncertainty. Therefore, the uncertainty of  $V_{n+1}$  is a function of two random variables, v and  $V_n$ , undergoing nontrivial nonlinear transformations. The unscented transformation (UT) [3,5] is employed as an efficient way to estimate the variance of  $V_{n+1}$ . The UT deterministically selects samples from the distributions of v and  $V_n$  and estimates the variance from the output statistics of the surrogate evaluated at these points.

The surrogate appears to reproduce the RELAP5 results with reasonably accuracy for all of the sequences including the cross-validation cases. The surrogate trajectories are smooth curves compared to the noisy RELAP5 data. Portions of the RCS remain voided and the localized TH conditions in the core where the single-phase flow is transitioning to two-phase flow display high frequency fluctuations due to the low pressure and low flow rate conditions during recirculation. The detailed RELAP5 UCN3&4 model can predict the oscillatory conditions evident in the water level data, whereas the surrogate was derived from a few simple variables representing the mass and energy flux boundary conditions of the RCS. The surrogate was intended to predict the macroscopic behavior of the system and was capable of learning this behavior from noisy data, a clear benefit of the ACE algorithm. The surrogate did not include any input variables that describe the heat transfer and condensation or superheating of steam in the steam generator of the intact loop.

#### 4. Dynamic Event Tree Application

In this section, the applicability of surrogates to dynamic PSA is demonstrated by studying a simplified DET of the recirculation phase. The transition from the injection phase to the recirculation phase at RAS time involves significant changes in the HPSI system configuration and uncertain conditions within the containment sumps. The DET specifically considers degradations to the HPSI system related to Generic Safety Issue 191, debris accumulation at the containment sump screens resulting in the loss of NPSH, and operator action time to diagnose and repair a failed HPSI pump. The fast computation time of the surrogate model allows the DET to be simulated by a direct Monte Carlo (MC) method. The MC solution serves as a benchmark to validate a newly proposed method using the UT to generate degraded component states and branch point times in the DET.

The initiating event for the DET is failure of HPSI pump B at the RAS time. HPSI pump A is assumed to have been successfully realigned to a containment sump and operates in recirculation mode. To account for possible degraded sump conditions, the available NPSH to pump A is assumed to be uniformly distributed U[7 ft,20 ft]. The flow rate of pump A is obtained from the NPSH curve for OPR-1000 HPSI pumps from [4]. The time for the operator diagnosis of the failed state of HPSI pump B and repairs is assumed to be normally distributed N[4500 s, 1800 s]. Once repaired and operating, the available NPSH for pump B is uniformly distributed U[7 ft, 20 ft]. The sump water temperature used to calculate  $h_p$  is assumed to be normally distributed N[345 K, 10 K]. These four variables reflecting an uncertain repair time, degraded sump conditions, and uncertain containment conditions are the input parameters to the DET.

The DET is evaluated using the MC method with 10,000 simulations by randomly sampling the distributions of the 4 uncertain variables. The surrogate is used to calculate the subcooled water level in the core for each sequence with  $w_p = w_{pumpA}$  for  $t < t_{repair}$  and  $w_p = w_{pumpA} + w_{pumpB}$  for  $t > t_{repair}$ . Each simulation is terminated at 12,000 s. Figure 9 shows 100 selected simulations. Each trajectory V(t) corresponds to a unique branch of the DET. The water level can vary by over 50% of the active core height during most of the transient, suggesting that the plant behavior can be highly variable even with 1 of 2 HPSI pumps always functioning within operational limits.

The DET is evaluated a second time using the UT method requiring only 9 simulations. Figure 10 shows the 9 UT simulations from which the mean and variance of the water level trajectories subject to the uncertainty of the 4 variables are estimated. The mean and variance are also calculated from the MC simulations, and Fig. 11 shows a comparison of the UT estimate to the MC benchmark. The UT and MC results are in close agreement. Clearly, performing 10,000 RELAP5 simulations is unreasonable so the surrogate is a useful

tool to facilitate direct MC simulation of DET and benchmark more efficient sampling methods such as the UT that would enable direct use of TH codes in dynamic PSA applications.



Fig. 9. 100 Monte Carlo simulations of repair of HSPI pump DET.



Fig. 10. Unscented transformation simulations of repair of HPSI pump DET.



Fig. 11. Monte Carlo vs. UT estimates of mean and variance for the repair of HPSI pump DET.

#### 5. Discussion and Future Work

A time-dependent surrogate model to predict core subcooling during the recirculation phase of a hot leg LBLOCA in the OPR-1000 has been developed. The surrogate assumed the structure of a general discrete time dynamic model and learned the nonlinear functional form bv performing nonparametric regression on RELAP5 simulations with the ACE The surrogate model input parameters algorithm. represent mass and energy flux terms to the RCS that appeared as user supplied or code calculated boundary conditions in the RELAP5 model. The surrogate

accurately predicted the TH behavior of the core for a variety of HPSI system performance and containment conditions when compared with RELAP5 simulations. The surrogate was applied in a DET application replacing computational expensive RELAP5 simulations allowing rigorous evaluation of the DET by MC methods and benchmarking of more efficient sampling methods.

The concept of surrogates and application to timedependent simulations of NPP TH behavior has been However, we recognize that the demonstrated. recirculation phase transient studied is well defined for the performance of one system, the HPSI system, and indirectly by containment systems. For more complex transients involving several systems or more sources or energy and mass flux such as heat removal through the SGs, more complex surrogates that can predict coupled TH behavior such as temperature, pressure, and loop mass flows will need to be developed, requiring a more systematic approach to identifying and defining input parameters for surrogate construction. Recent work has demonstrated fractional scaling analysis at the system level providing a framework identifying key TH relationships that drive the rates of change of system variables in NPPs [6]. Such methods may be useful for scaling data from TH code simulations during surrogate training allowing the flexibility of surrogates to learn more fundamental NPP behavior rather than system response to specific system configurations and initiating events.

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