



Japan Atomic Energy Agency

# An Integrated Approach to Source Term Uncertainty and Sensitivity Analyses for Nuclear Reactor Severe Accidents

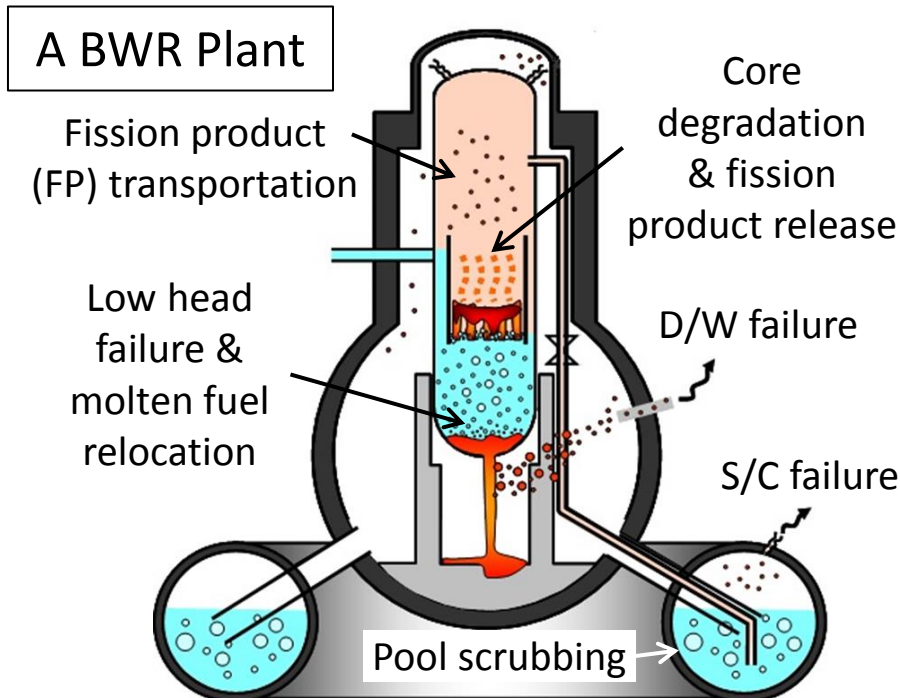
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# Introduction

- **Source term** (more sophisticated, FP): radionuclides, including physical & chemical forms, released to the environment during a severe accident.
- Source term directly affects the risk assessment of a NPP, including Level II & III PRA, and the planning of emergency preparedness & response.



Source term is simulated by using integral SA codes (MELCOR, THALES2), but **uncertainties** exist

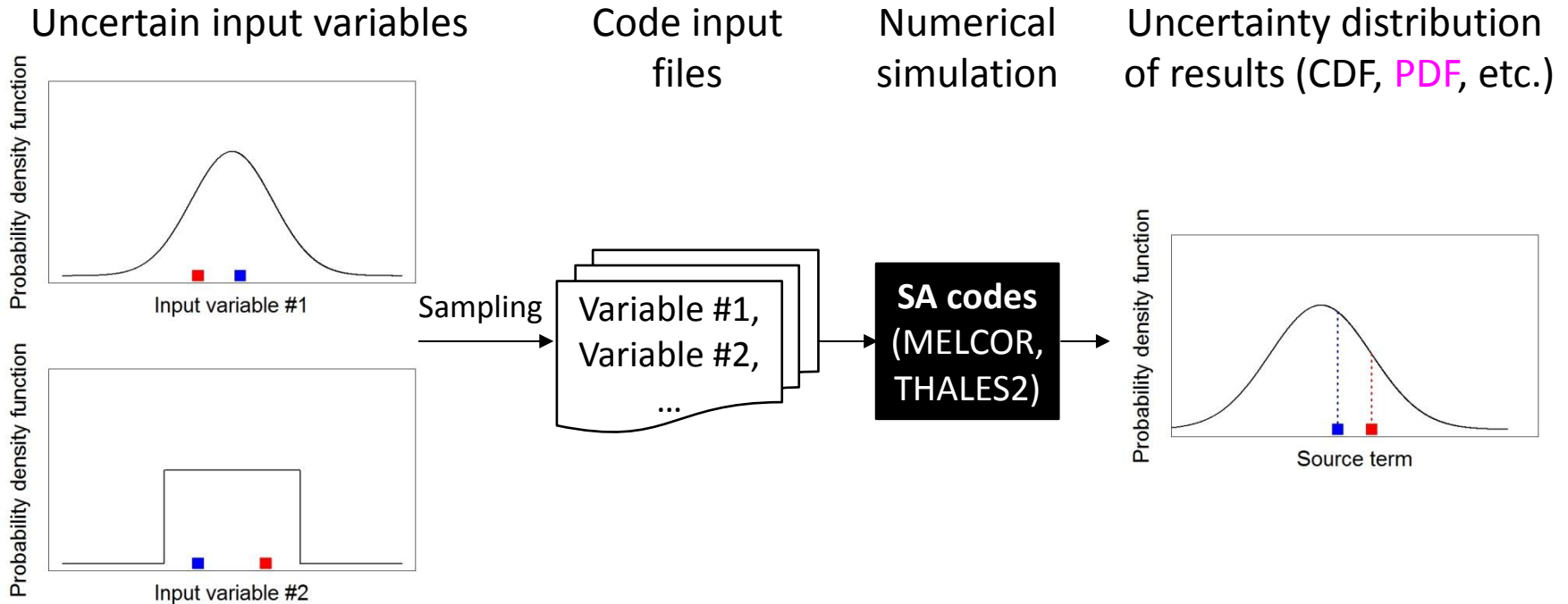


Uncertainty analysis quantifies the “error” in source term estimation



**Sensitivity** analysis finds what caused the source term uncertainties

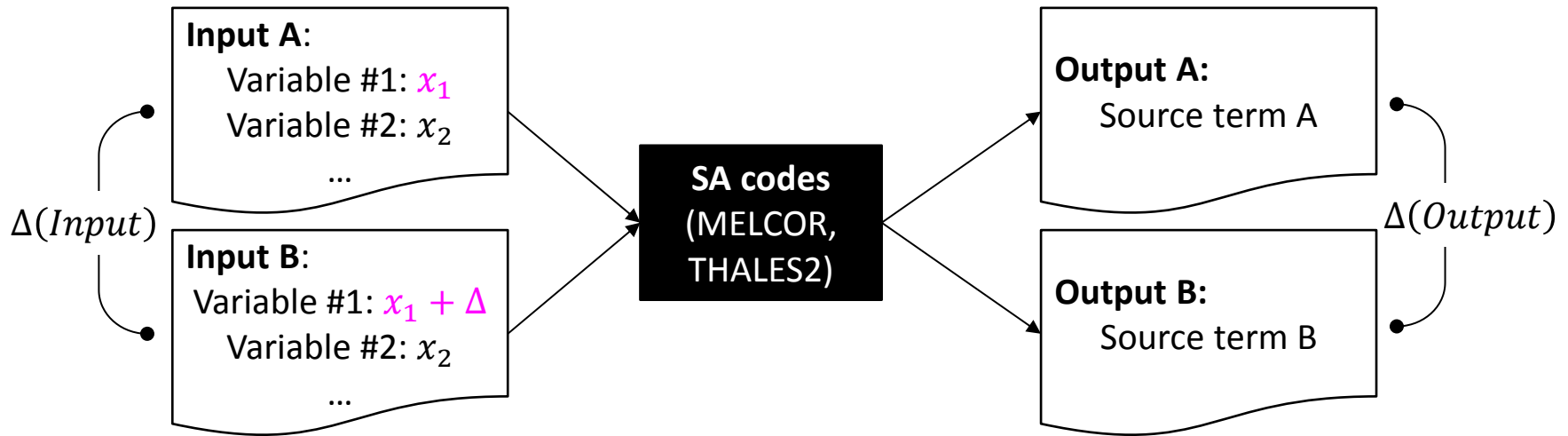
# Traditional Uncertainty Analysis



## Problems:

- How to select (screen) important uncertain input variables?
- Is there any necessary correlation (dependency) among these variables?
- How many times of code simulations are necessary?

# Traditional Sensitivity Analysis (Local)



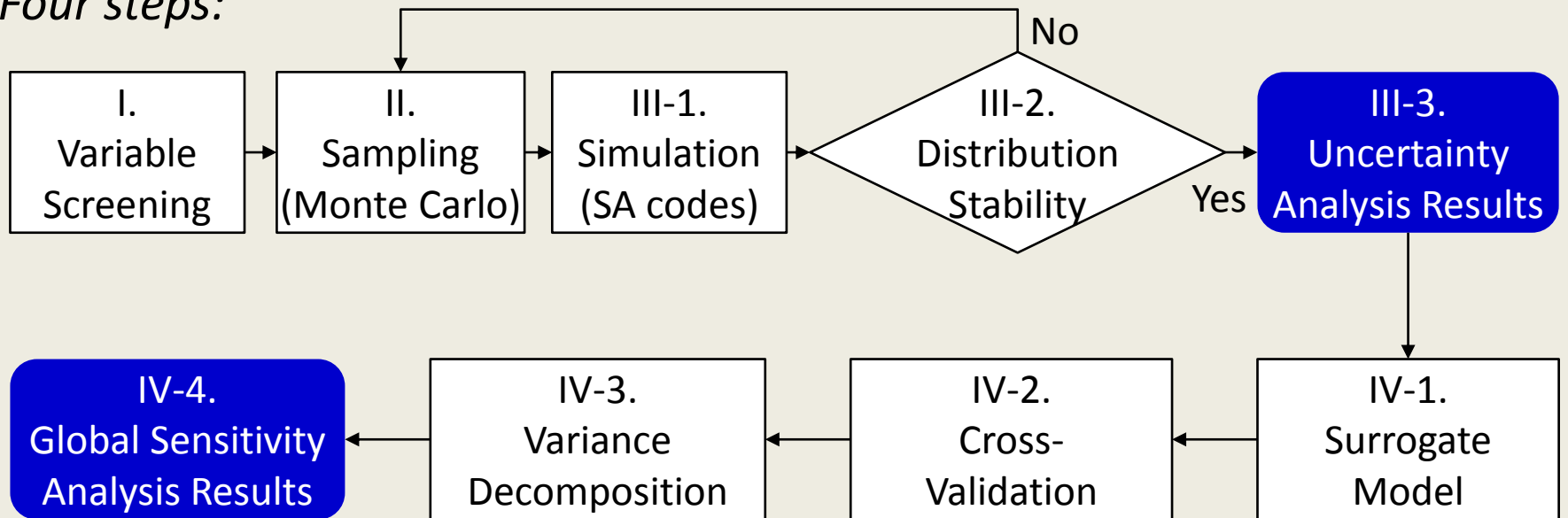
- For example, **local** sensitivity of Variable #1:  $S_1 = \frac{\Delta(\text{Output})}{\Delta(\text{Input})} = \frac{\text{Output B} - \text{Output A}}{\Delta}$

## One of problems:

- The setting of other variables will affect the result,  $S_1$ . It is called **interaction** between variables, but how to quantify it? (**Global** Sensitivity Analysis can be used to solve the problem.)

# Our Integrated Approach to U & S Analyses

*Four steps:*



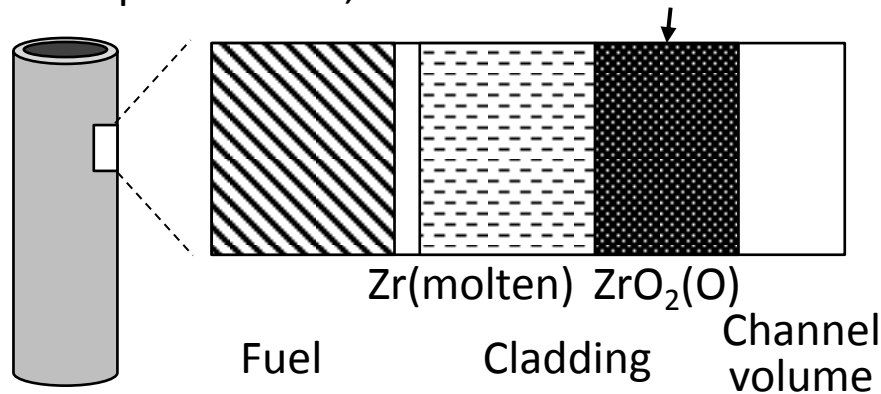
[To Summary](#)

# Uncertainty Analysis of Source Term

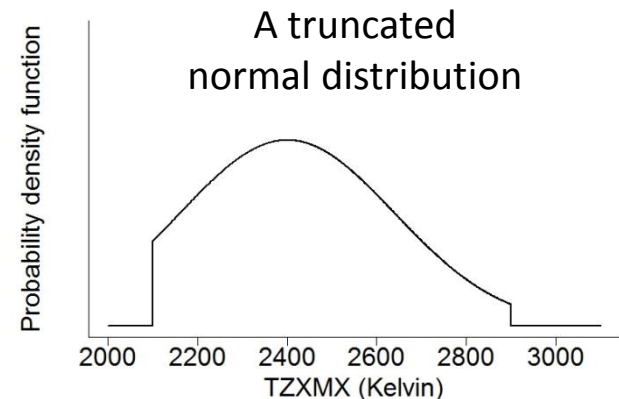
- The accident sequence similar to 1F2 (water injection & SRV operation, etc. fixed) is simulated by using MELCOR.
- Some severe accident phenomena related input variables are uncertain based on the current state of knowledge, whose influences on source term are concerned.

Totally, 27 uncertain input variables are regarded as potentially influential.

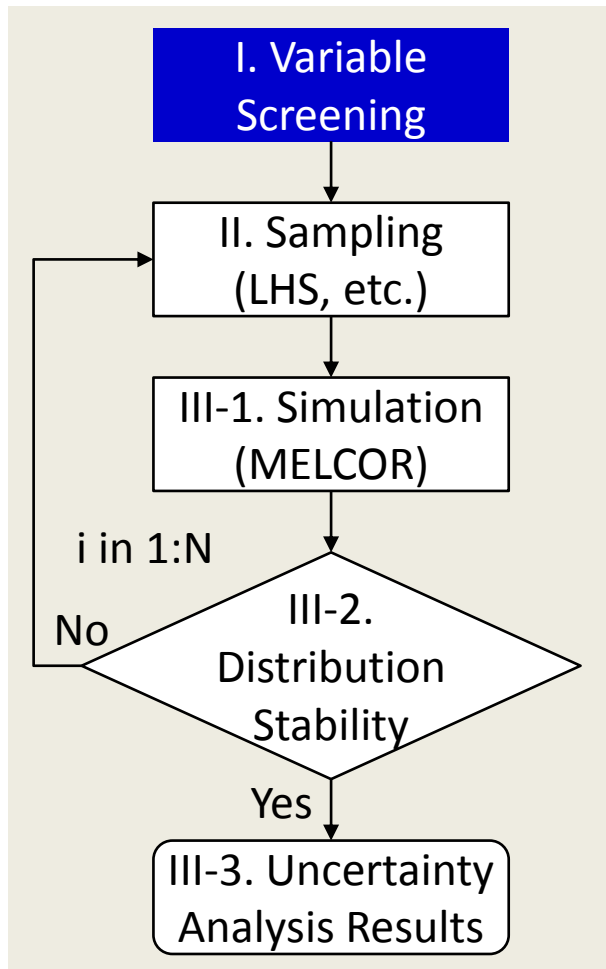
(1/27) TZXXM: Maximum  $ZrO_2$  temperature permitted to hold up molten Zr; MELCOR default value = 2400 K



Molten Material Holdup Model in MELCOR



# I. Uncertainty Analysis: Screening Method

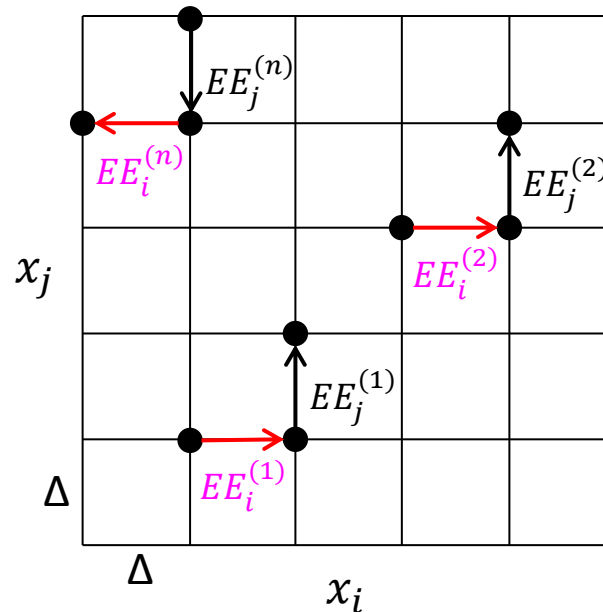


➤ Inputs: 27 → 10 (via screening analysis based on elementary effect method)

Elementary effect (EE) of an input:

$$EE_i = \frac{f(x_i + \Delta, \mathbf{x}_{\sim i}) - f(x_i, \mathbf{x}_{\sim i})}{\Delta}$$

$$\mathbf{x}_{\sim i} = [x_1, \dots, x_{i-1}, x_{i+1}, \dots]$$



Average sensitivity:

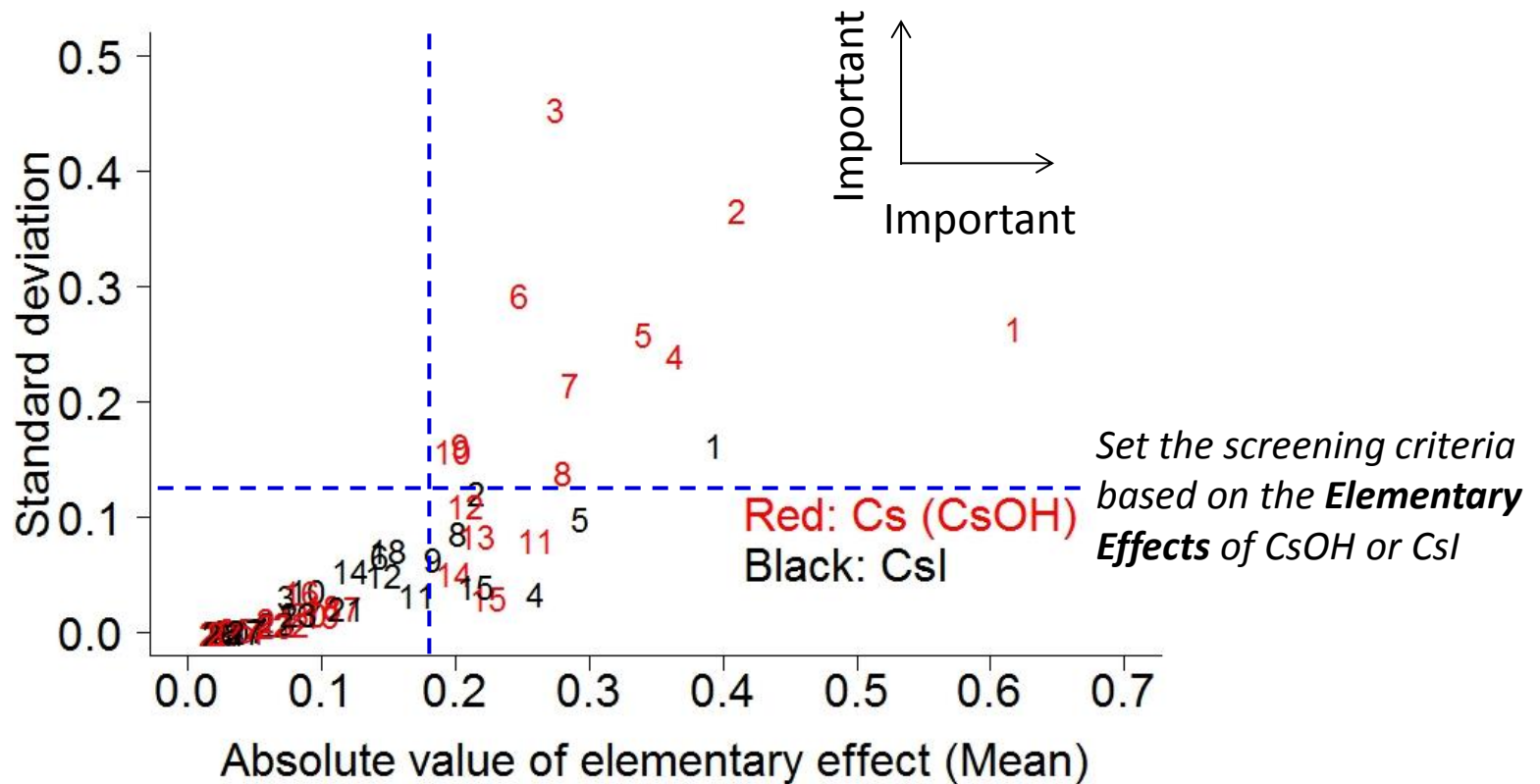
$$\mu_i = \frac{\sum_{k=1}^n |EE_i^{(k)}|}{n}$$

Interaction from other variables:

$$\sigma_i^2 = \frac{\sum_{k=1}^n (EE_i^{(k)} - \mu_i)^2}{n - 1}$$

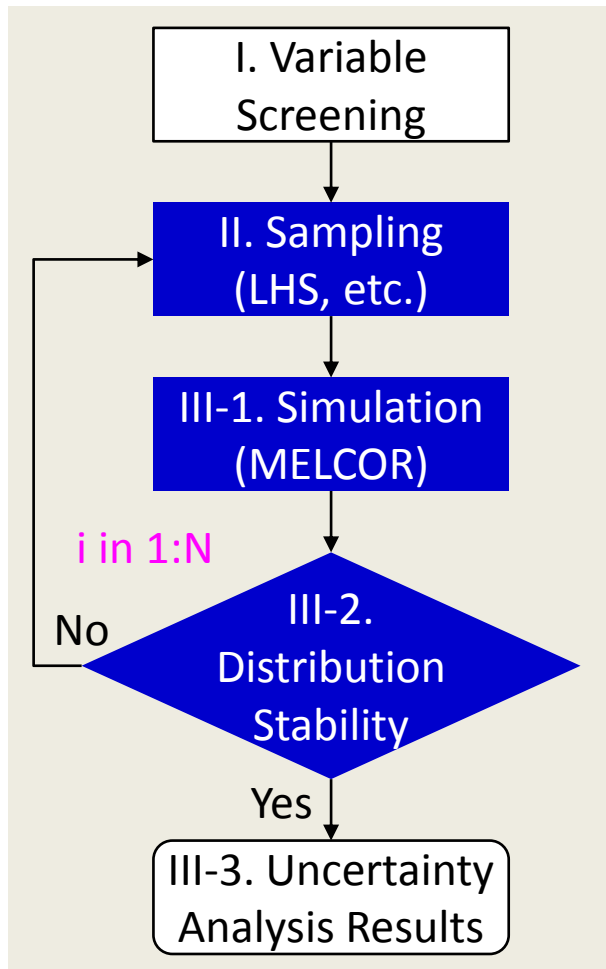
# I. Uncertainty Analysis: Screening Results

- After multiple (here, six) rounds of calculation, 10 relatively important variables are selected:

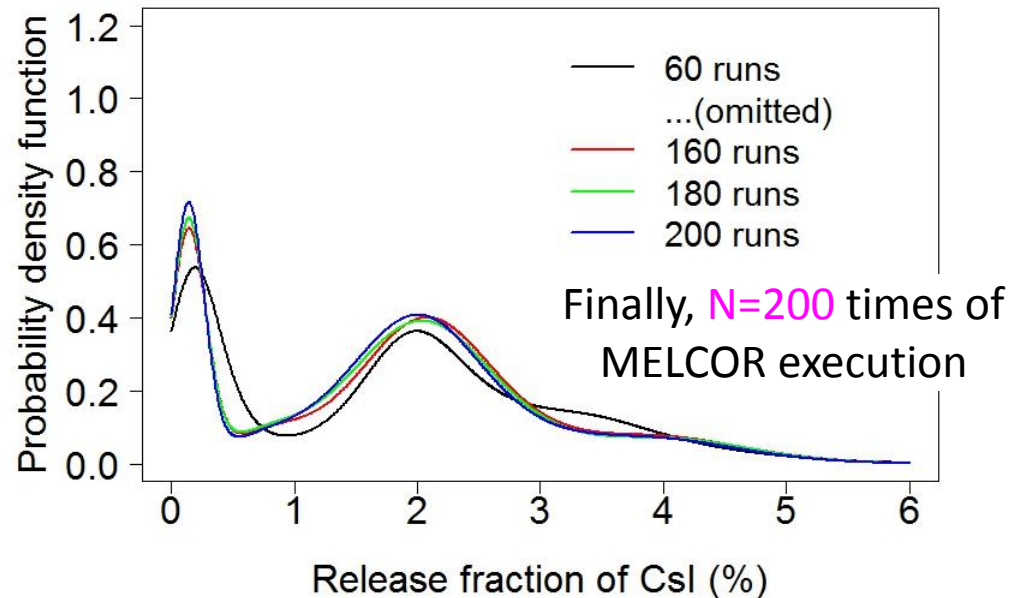




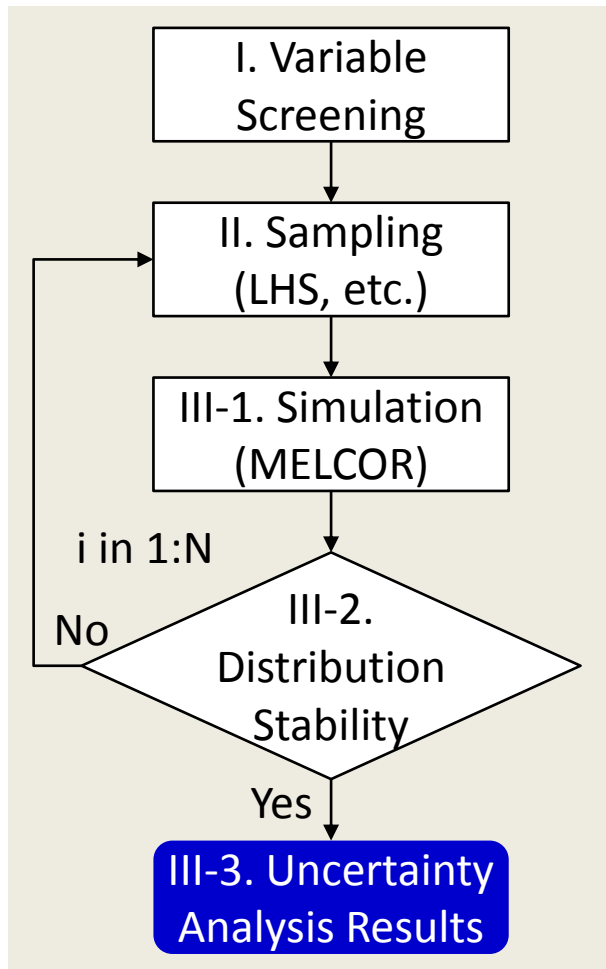
## II. ~ III-2. Sampling-Based Iterative Computation of Source Term



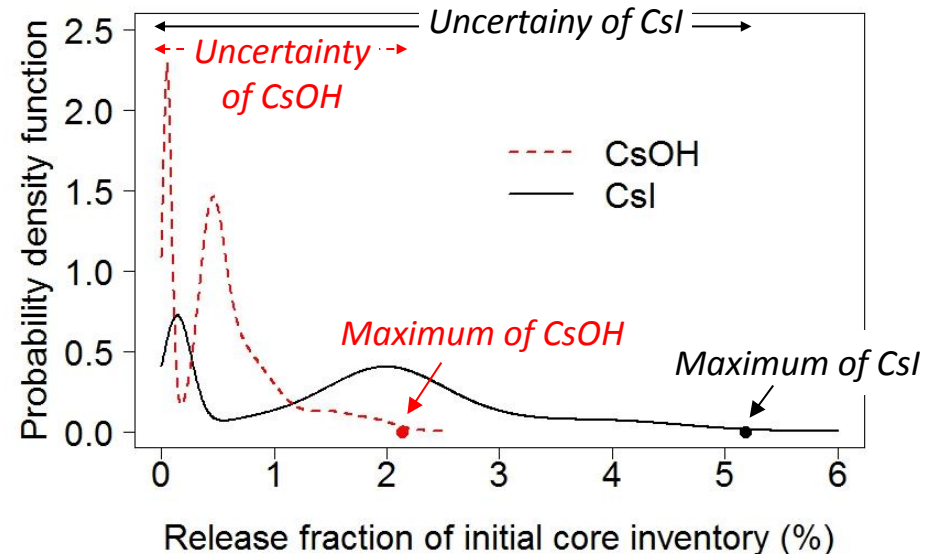
- Applied a method of Monte Carlo (Latin Hypercube sampling) with consideration of correlation among input variables;
- Keep iterating until probability density functions converge.



# III-3. The Results of Source Term Uncertainty Analysis



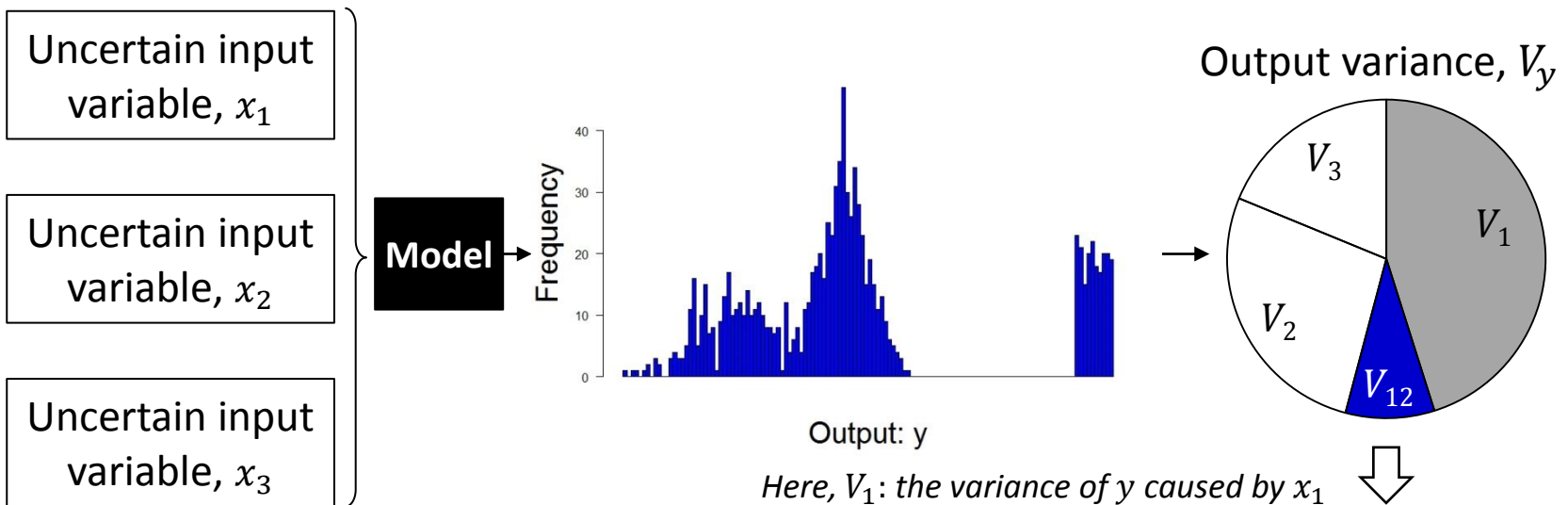
- After 200 MELCOR simulations, we obtained the probability distributions of representative source terms (CsOH, CsI, Ba, Te) released to the environment.



**Question:** Which input variables, with their uncertainties, are most influential for the source term uncertainties?

# Global Sensitivity Analysis via Variance Decomposition

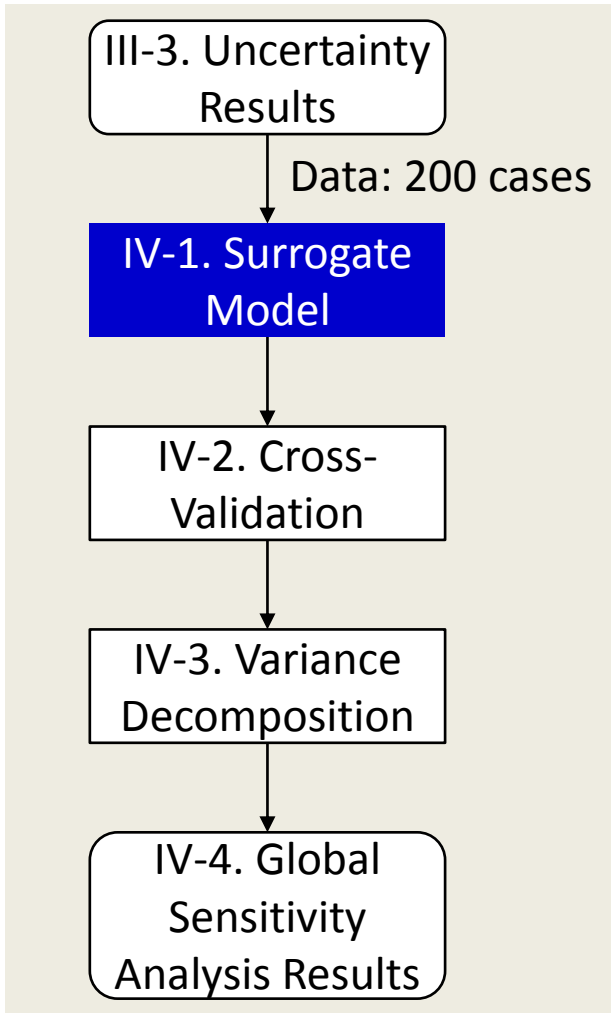
- The total uncertainty of Output  $y$ , can be decomposed based on the contribution from input variables,  $V_i$ , and their **interaction**,  $V_{ij}$ .



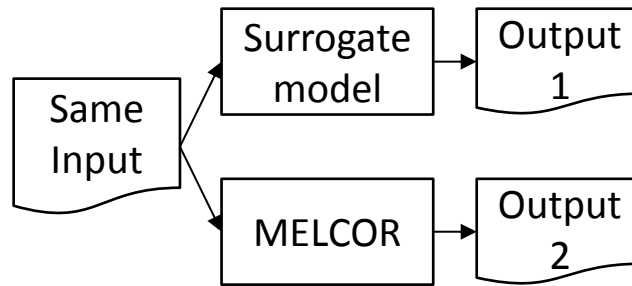
**Global Sensitivity Index (SI)** of input variable  $x_1$ :  $SI_1 = \frac{V_1 + V_{12}}{V_y}$ ;  $SI_1 > SI_2 > SI_3$

- The calculation of variance needs a lot of samples when input space is high-dimensional. It is **unaffordable (thousands of code executions)** by using complicated SA codes, MELCOR or THALES2.

# IV-1. Surrogate Model for the MELCOR Code



- The key step is to build a **surrogate model** (statistical model) to replace MELCOR, for the variance decomposition.
  - Use MELCOR simulation data to build the surrogate model (regression);
  - The computational cost of the surrogate model is low, so global sensitivity analysis is achievable.



## Basic Logic:

If Output 1  $\approx$  Output 2:  
Use the surrogate model instead of MELCOR  
Else:  
Execute more MELCOR simulations for surrogate model building

# IV-1. Build the Surrogate Model by using a Bayesian Nonparametric Method

- ① Data are not visualizable, “even messy”, for high-dimensional (10) inputs;
- ② When the predictability is not good, more simulation data are required, so the model structure will change;
- ③ We should avoid over-fitting and under-fitting.

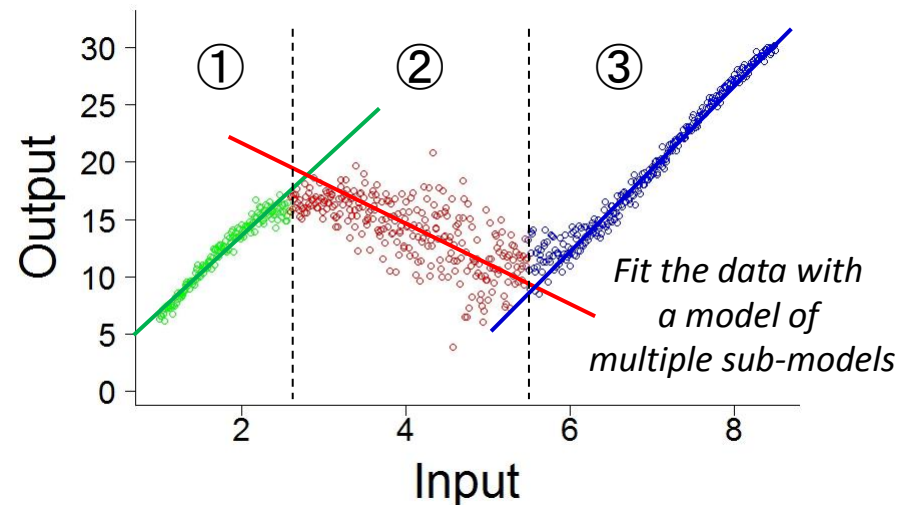
Why do we use DPM?

- An **infinite** mixture model for regression (a **Dirichlet Process Mixture** of Gaussians)

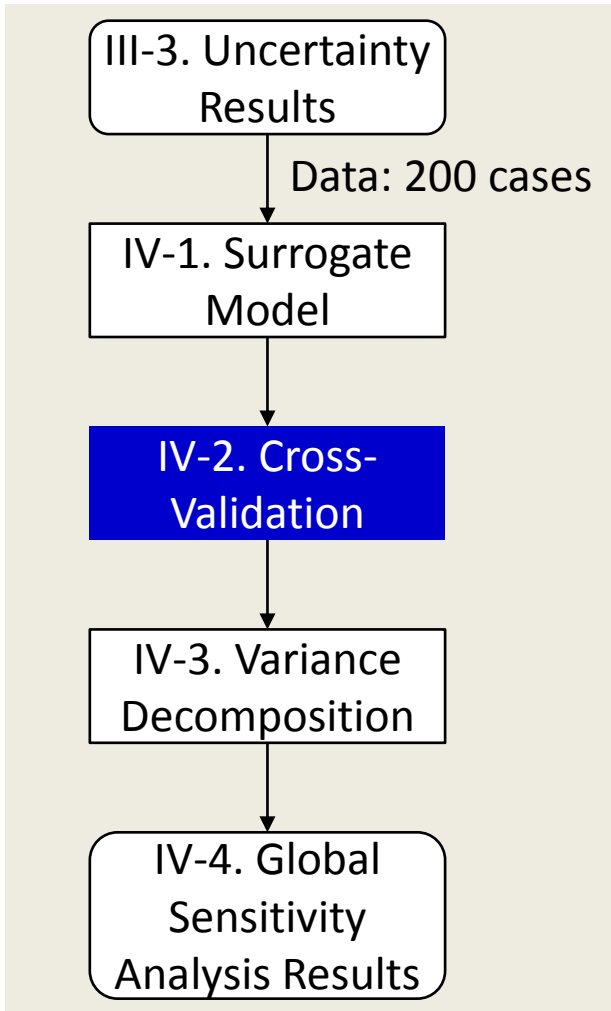
$$f(\mathbf{x}) = \sum_{k=1}^{K \rightarrow \infty} \pi_k(\mathbf{x}) N(\mu_k(\mathbf{x}), \sigma_k^2)$$

- By using DPM, the predictability of the surrogate model is good and can be used to replace the MELCOR code. The surrogate model structure can “**grow**” accordingly, when new data are available.

An example: mixture number,  $K = 3$ , is inferred (via MCMC Gibbs sampling), **NOT** determined beforehand. **Flexible!**

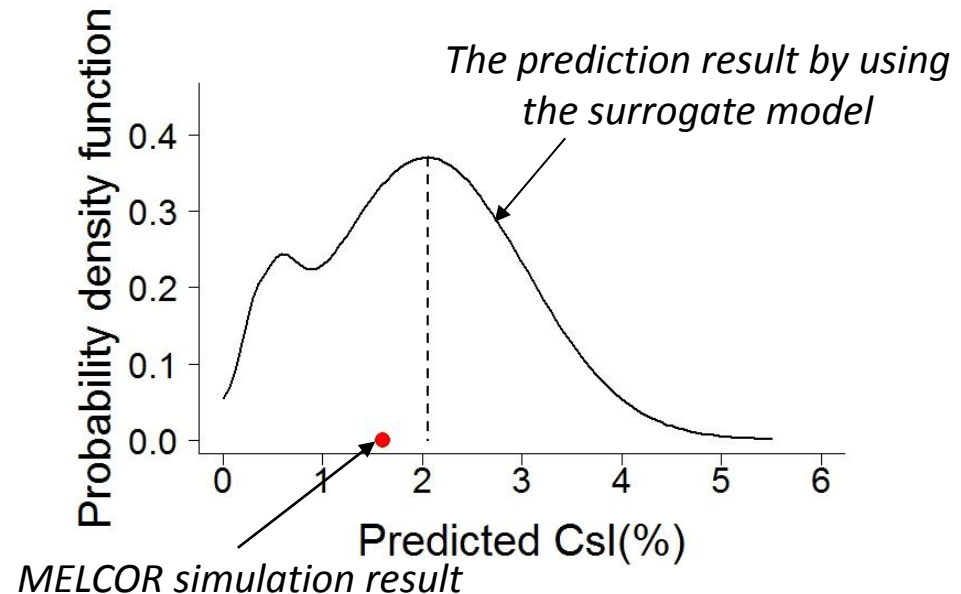


## IV-2. Validate the Surrogate Model



- Based on the input-output data from uncertainty analysis (200 code runs of MELCOR) , we use 190 to build the surrogate model and 10 for validating.

One example of the cross-validation



## IV-3&4. The Results of Global Sensitivity Analysis

- To calculate the global sensitivity index (SI), the surrogate model has been executed **21000** times, iteratively. (One execution of MELCOR code: 6 hours; that of the surrogate model: < 1 min)
- Most important variables can be identified and should be studied for the reduction of uncertainties in source term estimation.

Input variables	SI	Rank (GSA)	Associated Phenomena	Rank (EE)
TZXMV	0.802	1	Molten Zirconium holdup	4
DELDIF	0.736	2	Aerosol dynamics	7
TRDFAI	0.725	3	Fuel rod degradation	1
SC7155 (1)	0.556	4	Pool scrubbing	3
SC7160	0.518	5	Chemisorption	5
Others (6-10)				$(\mu + \sigma^2)$

*\*More information about the ranking of sensitive variables and surrogate model construction:*

(1) X. Zheng, et al. *Journal of Nuclear Science and Technology*, 53(3): 333-344 (2016)

(2) X. Zheng, et al. *Reliability Engineering and System Safety*, 138: 253-262 (2015)

# Summary

- An [integrated approach](#), to the source term uncertainty and global sensitivity analyses, has been successfully developed.
- By using a Bayesian nonparametric model, a **surrogate model** is successfully built to replace the **MELCOR** code for the global sensitivity analysis.
- As a conclusion, the dominant variables for the uncertainty in source term estimation can be identified. Further efforts need to be spent on the reduction of uncertainties on the variables (coefficients) and related models, which were generally simplified in the SA codes.
- In future, the approach will be applied to scenario uncertainty analysis for severe accident research, and all methods including the surrogate model would be very useful for nuclear PRA research.



# THANK YOU FOR YOUR COMING AND KIND ATTENTION

Attached materials:

- (1) List of important MELCOR input variables
- (2) 日本語版の発表資料

# Appendix. List of Important MELCOR Input Variables

No.	Input Variables	Associated Phenomena	Description
1	TZXXM	Molten material holdup	Maximum ZrO <sub>2</sub> temperature permitted to hold up molten Zr (default = 2400.0 K)
2	DELDF	Aerosol dynamics	Diffusion boundary layer thickness for aerosol dynamic processes (default = 1.0E-5 m)
3	TRDFAI	Fuel rod degradation	Temperature at which oxidized fuel rods can stand when unoxidized Zr is absent from the cladding (default = 2500.0 K)
4	SC7155 (1)	Pool scrubbing	A variable used to calculate the decontamination factor for the particle impaction process, when the Stokes number is small (default = 1.79182)
5	SC7160 (1,1)	Chemisorption	Used to calculate the chemisorption rate for CsOH and CsI on the surface of stainless steel (default = 0.139 m/s)
... (6-10)			