Thesis subject:
Reliability enhancement of severe accident computer codes by data assimilation and sensitivity analysis.

Context

The frame of the proposed thesis work concerns the simulation of severe accidents in light water nuclear reactors. In an accident situation, nuclear fuel can melt and interact with surrounding structures to form a corium pool in the reactor core and then, after relocation, in the bottom of the vessel. In case of vessel failure, the corium can then relocate in the reactor pit, reach the basemat and interact with the concrete that constitutes it. In the presence of water, the interaction between corium and coolant can lead to a steam explosion, an energy event that may compromise the integrity of the containment.

Simulation software (or calculation codes) for severe accidents improve the safety of nuclear reactors by providing information to help predict the failure of barriers or safety systems.

The simulation of the corium path in the reactor can be done by two approaches: either an approach focused on a particular step of the path, or a global approach allowing the coupling and interaction between the physical phenomena present in several steps of the path. The codes dedicated to the first approach are generally meshed (or at least partially) with a model of the physics involved described in the meshes in the form of a closing law (subgrid modeling). We can for example mention MC3D, which simulates the corium water interaction and steam explosion. For the second approach, the codes, such as PROCOR, consist of a set of models (integral or limited in the mesh size fineness) describing each step of the corium path during the accident. These models can then be assembled to describe the sequence of steps, taking into account the transient aspect of physics.

The models of these codes and the way they are coupled generally use parameter sets adjusted on experimental results or on DNS-like fine calculation results.

Objective and methodology

The objective of this thesis is to build a methodology to quantify and increase the accuracy of these calculation codes. To do this, data assimilation and sensitivity analysis are considered.

The models of the calculation codes are parametric with input parameters (defining the simulation desired by the user) and with model parameters (specific to each model). Thus, improving the accuracy of model parameter values contributes to improving the accuracy of calculation codes.

The simulation results of these codes can be scalar or functional (time or space dependent).

The main steps envisaged for the thesis work are presented below.

First, a ranking of model parameters will enable to reduce the size of the parameter space. For this purpose, screening methods may be used. Among those commonly used, we can mention Morris'[1], which makes it possible to distinguish between non-influential parameters from those with a linear effect and those with a non-linear effect and/or in interaction with other parameters. It has the drawback of requiring a specific experimental design, OAT (One At a Time). Another possible screening method based on dependence measures [2] does not require any specific experimental design. A design with good space occupancy properties (e.g. low-discrepancy LHS) can then be used for parameter screening and later reused for other tasks such as surrogate model construction.

Then, a calibration methodology of the model parameters will have to be implemented. For this purpose, data assimilation methods may be used to quantify the difference between the software simulations and the reference results, experimental or derived from DNS-type fine calculations, in order to ultimately define a set of adjusted parameters that minimizes this difference. These methods also have the advantage of allowing any new results to be assimilated that enrich the reference database (experimental or DNS) and thus take into account new knowledge in the physics of the involved phenomena. To achieve this assimilation, Bayesian calibration, which has undergone significant growth in recent years [3,4], could be considered.

Depending on the complexity and computational time, the use of surrogate models may be necessary. Their construction will be based on a reduced number of parameters, selected at the end of the screening stage. The methods of building machine learning-based surrogate models have evolved considerably in recent times. Among these, we can mention neural networks, random forests [5], chaos polynomials or Gaussian process Kriging.

When setting up the calibration methodology, particular attention will be paid to the propagation of uncertainties. In addition to obtaining the uncertainties of the calibrated parameters, a model error estimate could be considered [4].

Finally, a sensitivity analysis of the results of the simulation codes to the input parameters, globally and for each model, will also contribute to increasing the accuracy of the results. Indeed, this sensitivity analysis makes it possible to identify the most influential parameters and models, on which a better knowledge (through new studies, new experiments...) has the greatest effect on the accuracy of simulation results.

Sensitivity analyses, based for example on the calculation of Sobol's global sensitivity indices [6], generally require a large number of samples to converge, again involving the construction and use of surrogate models.

Application calculation code

The application of the methodology will be implemented for the simulation of the Corium Water Interaction which uses the MC3D calculation code, with the aim of being as generic as possible in order to be usable and easily transposable to other severe accident calculation codes.

This choice lies in the fact that corium-water interaction is a complex phenomenon, highly non-linear, with non-monotonic results, involving many mechanisms interaction and that, in terms of safety, it can potentially compromise the integrity of the reactor containment.

MC3D [7], is a multiphase, multicomponent Eulerian code, describing the interactions between molten corium and liquid water in a discretized domain with a structured 3D mesh. Two modules are available to simulate each of the two phases of corium-water interaction. The first is dedicated to the premixing phase during which the corium jet is coarsly fragmented into millimeter drops as it enters the water. Temperatures are so high that the water enters a film boiling regime around the corium. The second is dedicated to the simulation of the explosion triggered by a local destabilization of the vapor film surrounding the corium drops. Those drops are finely fragmented (fragment size in the order of 50µm) which highly increases the exchange surface and the generation of vapor causing a pressure wave. This is similar to an explosion that, when generated, spreads through the coarse mixture of corium and water drops, fragmenting the drops as it passes and sustaining the explosion. In the code, physics is described by sub-mesh models.

Experimental data

The experimental data base for this phenomenon consists of about fifteen tests performed at different scales on several facilities. Among the tests that can be used as references for the calibration of MC3D models there are those performed on the FARO[8] and KROTOS[9][10] installations.

A master 2 internship is in progress to exploit and analyze the available experimental results and organize them for the calibration step.

Among the input parameters on which the sensitivity analysis will be carried out, the physical properties of corium are of particular interest because of their influence that was highlighted during a preliminary study and because of the ability of the CEA to perform new measurement with its experimental facilities. The goal is a better use of these properties and a precise identification of the needs for simulation (which will allow supporting for measurement campaigns proposals, for example with the CEA experimental platforms VITI [11] or ATTHILA[12]).

Use and capitalization of the thesis results

The results of this thesis will contribute to the improvement effort of the severe accident simulation.

The surrogate models developed during this thesis could be used as models in the PROCOR platform [13]. This platform, developed at the CEA, capitalizes the modeling of corium propagation under the form of a set of physical models that can be assembled in specific applications dedicated to the desired simulation (e.g. for a given reactor type and a defined propagation step). For a phenomenon to be simulated, there can be several available models; the choice of model to use depends on the application or the user's choice. Currently, the platform includes a basic statistical module using URANIE [14]. The methods developed in this thesis will be capitalized in this statistical module.

At the end of this thesis, the candidate will have developed skills (in probability, statistics, physics of severe accidents...) that will allow him to apply for a research or R&D position.

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