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Validation Methodology applied to SIMMER code for Fusion Applications

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Validation Methodology applied to SIMMER code for Fusion Applications

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The Verification and Validation (V&V) activity of the modified version of SIMMER-III code for fusion applications has been carried out applying a standard methodology for code validation. The methodology is based on a three-steps procedure and through qualitative and quantitative evaluations: 1) the initial condition results, 2) the reference calculation results, and 3) the results from sensitivity analyses. The qualitative accuracy evaluation is performed through a systematic comparison between experimental and calculated time trends based on the engineering analysis, the resulting sequence of main events, the identification of phenomenological windows and of relevant thermo-hydraulic aspects. Finally, the accuracy of the code prediction is evaluated from quantitative point of view by means of selected, widely used, figures of merit. The methodology was applied to the LIFUS5 campaign, available in literature. Post-test analyses highlighted open issues of test execution and of experimental data, as well as code limitations and capabilities.

Keywords: SIMMER, Chemical Reaction, Deterministic Safety Analysis, WCLL Breeding Blanket, Code Validation.

1. Introduction

The reliability of qualified system code for deterministic safety analysis of in-box Loss of Coolant Accident of the Water Cooled Lithium Lead breeding blanket concept [1], [2] is of primary importance, in view of the evaluation of accidental consequences and mitigating countermeasures. The modified version of SIMMER code for fusion application, which implements the PbLi/water chemical reaction, has been developed by University of Pisa and ENEA C.R. Brasimone [3] and currently is under validation process [4], [5].

2. Procedure for code validation

The paper presents the application of a standard methodology for the “SIMMER-III Ver. 3F Mod. 0.1” code validation, the version of SIMMER-III modified for fusion application implementing the PbLi/water chemical reaction model [3]. The flow chart of the procedure is shown in Fig. 1 and hereafter described [6], [7].

The qualified nodalization input deck depends on several aspects:

- Code models. The information is available by the user manual and by the guidelines for the use of the code. They take into account the specific models, limits and assumptions of the code;
- User experience and capability. The user’s knowledge about the code is useful for the modelling phase;
- Facility geometry. The main geometrical dimensions of the facility are derived from the experimental database. This information should be derived from official document and traceability of each reference should be maintained.

Boundary and initial conditions of the considered experiment (i.e. input data for the reference calculation) may be changed within their uncertainty ranges in order to get the reference calculation; if a user choice is introduced (e.g. changes in nodalization detail due to lack of experimental data, misinterpretation of test, deficiency of geometrical information) its validity and acceptability must be checked by repeating the nodalization qualification process.

Then, a three-step analysis is pursued as a part of the code assessment process:

1. Initial condition results at injection time;
2. Reference calculation results;
3. Results from sensitivity analyses.

Step 1 constitutes part of the assessment process being relevant for the characterization of the thermal-hydraulic conditions at the beginning of the experiment. The reference calculation results (step 2) are those achieved from the qualified nodalization. Sensitivity analyses (step 3) are carried out to demonstrate the robustness of the calculation, to characterize the reasons for possible discrepancies between measured and calculated trends that appear in the reference calculation, to optimize code results and user option choices and to improve the understanding of experimental data.

The analysis of results is based on the comparison between measured and calculated trends or values and it is performed through 1) qualitative and 2) quantitative evaluations. A comprehensive comparison between measured and calculated trends or values is performed and analyzed based on qualitative engineering judgments, and quantitative evaluation of calculated-experimental discrepancies, including the following steps:

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a) analysis of code results and comparisons between experimental and calculated time trends on the basis of the selected variables;

b) evaluation of quantities relevant for the assessment of phenomena/processes and for the safety [6], [7], including the resulting sequence of main events;

c) evaluation of the accuracy based on selected figures of merit [8]-[10].

The qualitative accuracy evaluation is based upon a procedure consisting in the identification of phenomenological windows and of the RTA (relevant thermal-hydraulic aspects) [6], [7]. It essentially derives from a visual observation of the experimental and predicted trends. Then, the parameters characterizing the RTA (SVP = Single Valued Parameter, TSE = parameter belonging to the Time Sequence of Events, IPA = Integral Parameter, NDP = Non Dimensional Parameter) are quantified, giving information about the discrepancy between experimental and calculated results:

- Excellent (E): the calculation result is within experimental data uncertainty band. The code predicts qualitatively and quantitatively the parameter;
- Reasonable (R): the calculation result shows only correct behavior and trends. The code predicts qualitatively but not quantitatively the parameter;
- Minimal (M): the calculation result lies within experimental data uncertainty band and sometimes does not have correct trends. The code does not predict the parameter, but the reason is understood and predictable;
- Unqualified (U): the calculation result does not show correct trend and behavior, reasons are unknown and unpredictable. The code does not predict the parameter and the reason is not understood.

The qualitative analysis is a necessary prerequisite to the application of the quantitative analysis, to avoid misinterpretation due to compensation of errors. Quantitative accuracy evaluation can be defined as a systematic analysis of the deviation of the predicted target variables with respect to the corresponding measured values. Therefore, it plays a relevant role for quantify the accuracy of a code, thus the reliability and the capability in predicting parameters relevant to safety.

The statistic approach is based on time-averaging deviations of selected statistical parameters [8]. The starting point is the definition of the following equation:

$$DEV1_{i,t} = c_{i,t} - e_{i,t} \tag{1}$$

which is simply the difference between calculated and experimental value (*c* and *e*, respectively), for each location and for each time value. Both the calculated and the measured values must be "aligned" on the same time vector, usually this is not the case, because the frequencies of experimental data acquisition and code results are most likely to be different.

Once the DEV1 deviations have been calculated, they can be "integrated" over the time interval (arbitrarily specified, depending on the test) using the following equations. This leads to the three deviations DEV2: the first one represents the accumulative error and will come out with a positive value if the local perturbation has been over-predicted and vice versa; the second is just summing-up the absolute deviation and will always be non-negative; the third is a root mean square deviation, which enhances the contribution due to the large deviations.

$$DEV2\_SIGN_i = \frac{1}{t_N - t_0} \cdot \sum_{k=1}^{N} DEV1_{i,t} \cdot \left(t_k - t_{k-1}\right) \tag{2}$$

$$DEV2\_ABS_i = \frac{1}{t_N - t_0} \cdot \sum_{k=1}^{N} \left|DEV1_{i,t}\right| \cdot \left(t_k - t_{k-1}\right) \tag{3}$$

$$DEV2\_RMS_i = \sqrt{\frac{1}{t_N - t_0} \cdot \sum_{k=1}^{N} \left(DEV1_{i,t}\right)^2 \cdot \left(t_k - t_{k-1}\right)} \tag{4}$$

Another methodology suitable to quantify code accuracy (FFTBM approach) was developed at the University of Pisa [9], [10]. It consists of performing a discrete Fourier transform on both the experimental and the calculated time history of a given key parameter (over a specified time interval, and filtering the frequencies above a specified threshold), then comparing the resulting amplitudes in the space of frequencies. In particular, with reference to the error function, $\Delta F\left(t\right) = Fcalc\left(t\right) - Fexp(t)$, the method defines two values characterizing each calculation:

- A dimensionless average amplitude

$$AA = \frac{\sum_{n=0}^{2m} \left|\tilde{\Delta F}(f_n)\right|}{\sum_{n=0}^{2m} \left|\tilde{F}_{\exp}(f_n)\right|} \tag{5}$$

- A weighted frequency

$$WF = \frac{\sum_{n=0}^{2m} \left|\tilde{\Delta F}(f_n)\right| \cdot f_n}{\sum_{n=0}^{2m} \left|\tilde{\Delta F}(f_n)\right|} \tag{6}$$

The most significant information is given by the factor AA, which represents the relative magnitude of the discrepancy deriving from the comparison between the addressed calculation and the corresponding experimental trend (AA=1 means a calculation affected by a 100% of error). The WF factor characterizes the kind of error, because its value emphasizes whether the error has more relevance at low (small value of WF) or high frequency ones (large value of WF). The higher is the weighted frequency, the more relevant is the contribution of the high frequencies to the average amplitude. The two resulting factors AA and WF are a quantification of the code results accuracy, but obviously, they acquire a practical and understandable meaning only when they are compared against some analogous factors. For instance they can be compared with the same quantities coming from different calculations (for a code-to-code comparison) or with reference values (e.g. “acceptability thresholds”).

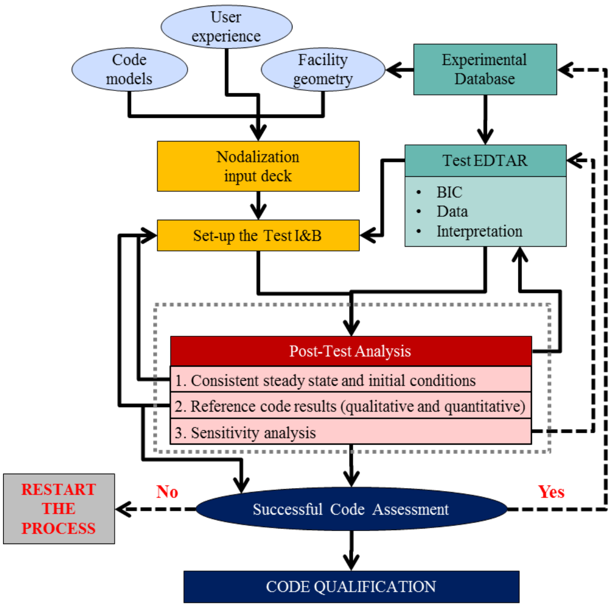

Fig. 1. Methodology for SIMMER code validation.

This approach is commonly applied to system code validation in nuclear reactor safety [11] and to relevant key parameters such as pressures in specified volumes, inventories, temperatures at given locations, etc., for which acceptability threshold may be available. The application of FFTBM to these kinds of interaction phenomena is pioneering. Nevertheless, it brought further contribution to the SIMMER-III code accuracy quantification, helping identifying most accurate code results, code models, and helping in experimental test comprehension.

Once the results of the post-test analyses are satisfactory for a selected test from both qualitative and quantitative accuracy evaluation, the validation process is applied to another test, maintaining the qualified nodalization and changing the initial and boundary conditions. If the results are not fulfilled, the process must restart.

The established standard methodology for code assessment was applied to validate SIMMER-III code against the experimental campaign on LIFUS5 performed during ’00 at ENEA CR Brasimone [12], [13].

3. Description of LIFUS5 experiments

3.1 Facility description

LIFUS5 facility, extensively described in literature [12], [13], was designed and operated at ENEA CR Brasimone to experimentally investigate the consequences of LOCA accidents in liquid metal pools. The reaction vessel S1 contained a mock-up of U shaped cooling tubes, as foreseen in previous design of WCLL BB for DEMO [14]. The water injection device was placed in the bottom of S1 below the tube bank sector and had an orifice diameter of 4 mm. Several pressure transducers (PT) and thermocouples were placed both in S1 and in the expansion vessel S5 to follow the pressure and temperature evolution during the interaction.

3.2 Tests description and open issues

Before the execution of a test, vacuum was generated between the valve V14 and the water injector. At the start of the test, valve V14 opened and hot pressurized water was discharged from the water tank S2 to S1 through the injection line. The water injection pressure was fixed and kept as constant as possible through a constant pressurization of the vessel S2. Then, the injection was interrupted closing the valve. The main operating conditions of each Test# are summarized in Table 1. On the basis of the review of available documents and of the validation activity ([4], [5], [12], [13]), the knowledge of the execution of the experiment is affected by uncertain data in relation to:

- Layout of the injector device and relative position in respect to the U-tube mock-up. No geometrical drawings or dimensional information was found in literature.
- Injected mass of water. No mass flow meter was installed in the injection line, therefore the amount of injected water was estimated by the experimentalists a posteriori. No accuracy is reported in literature, as well as no reference on the procedure used for the evaluation.
- Position of PT3. From the original drawing, PT3 was installed in the ascendant pipe of the vacuum line. Therefore, it is possible that the pressure recorded by PT3 was affected by vapor bubble formation, PbLi plugs, or PbLi drops which fall down and vaporize the water in the injection line, causing the increase of pressure recorded by the PT.

4. LIFUS5 SIMMER-III analyses

4.1 Facility nodalization

The nodalization of LIFUS5 by SIMMER-III code [15] is developed in 2D axisymmetric geometry (R-Z), despite the limitation of representing the asymmetries of LIFUS5 facility. In fact, the injection device and the tube bundle are not placed along the central axis of S1, but in one of the sectors limited by plates, while the expansion tubes are one for each sector. Therefore, assumptions were made in order to model this asymmetric layout. This implies that the user effect due to modeling choices and code options selections are relevant for the results of simulations. The nodalization set up for the reference calculation is shown in Fig. 2.

The geometrical domain is obtained by 11 radial and 47 axial mesh cells. The overall volume of the model is obtained rotating the 2D SIMMER domain along the axis of symmetry. The reference mesh cells used for the analysis and the comparison with experimental data are highlighted in yellow and are (6,4), (6,7) and (6,10) for the pressure in the reaction vessel S1 and (5,47) for the pressure inside the expansion vessel S5. The correspondence of main dimensions of LIFUS5 and SIMMER-III nodalization is reported in detailed in [4].

The reference calculations start at t = 0 s, which represents the valve V14 opening. The injector break-up is simulated by the virtual wall disappearing, which recreates the 4 mm orifice. The time at which the injector breaks-up depends on the experimental data of the single Test#, as well as the time of the injection.

The boundary conditions, are applied at the injector device (I=1-3, J=1). In Tests#6-8 it is assumed to impose the pressure recorded by PT3, while in Tests#3-5 it is assumed a postulated time trend. Moreover, the injection water temperature specified by the Test#, and the continuous inflow of injected water are imposed at the same mesh cells. The initial conditions of pressure, temperature, filling level of lithium-lead in S1 and S5 are set coherently with the experimental data of each Test#.

These assumptions imply that the amount of injected water is not imposed but is calculated by SIMMER-III accordingly to pressure difference between the injector inlet and the reactor vessel. The flow is then controlled by the interaction phenomena between lithium-lead and water.

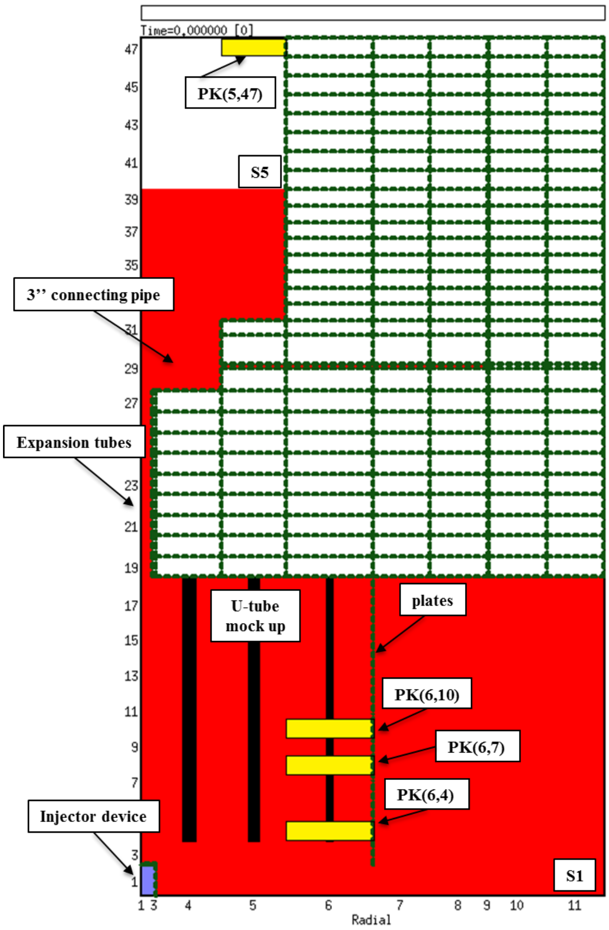

Fig. 2. SIMMER-III modeling of LIFUS5 facility and focus on reference mesh cells.

4.2 Post-tests analyses results

The code validation methodology was applied to all the Test# of LIFUS5 experimental campaign reported in Table 1. The obtained results, fully reported in Ref. [4], are here briefly described as example of the code validation methodology application.

The initial condition results (step 1 of the three-step procedure) highlight that during the vacuum line pressurization (from the V14 opening signal to the injector breaks-up), an early rupture of the injector cap occurred, leading to two-phase injection conditions. The calculations permit to improve the knowledge of tests procedure and tests operating conditions (i.e. the injected pressure trend and the pressure at which the injector cap breaks do not correspond to the design specifications).

Step 2 focuses on the reference calculation results, performed through qualitative and quantitative accuracy evaluations. From the former point of view, the code satisfactorily predicts the pressure trends in the reaction and expansion vessel (Fig. 3), and reasonably evaluates the temperature trends (Fig. 4). Considering the injected mass of water, it was calculated by experimentalists a posteriori because direct measurement was not available. The values have been reviewed and more realistic quantification is derived thanks the code simulations. Then, a verification of the code prediction is evaluated by means of engineering considerations. From the quantitative accuracy evaluation point of view, considering the peculiarity of LIFUS5 Tests# transient, their execution, and the availability of experimental data, the evaluation involves the pressures in reaction and expansion vessel. The results are reported in Table 2.

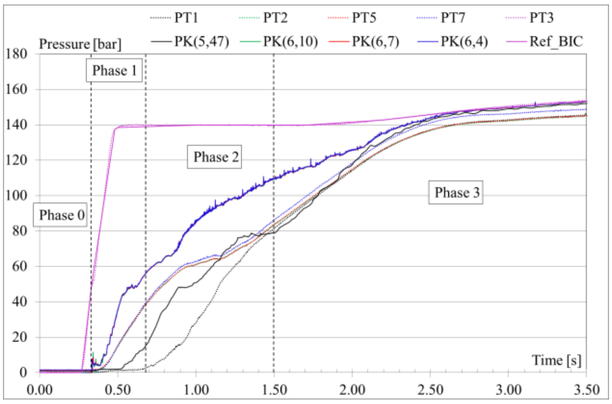

Fig. 3. T#8: pressure in S1 at different level PK(I=6, J=4-7-10), in S5 PK(5,47), and imposed (Ref_BIC), and comparison with experimental data (PT).

A series of sensitivity analyses (step 3) have been performed for each Test#, changing the initial and boundary conditions and the nodalization (i.e. modeling the U-tube elbow responsible to break the water jet). The results underline the importance of the correct knowledge of initial and boundary conditions (i.e. the pressure trend imposed at the injector, the temperature of the injected water, the free gas volume in the expansion vessel). Moreover, the results show that such kind of interaction phenomena is extremely complex to simulate because affected by a large number of parameters (i.e. interfacial area, dimensions of the vapor bubble, heat transfer coefficient, fragmentation mode due to the jet-breaking).

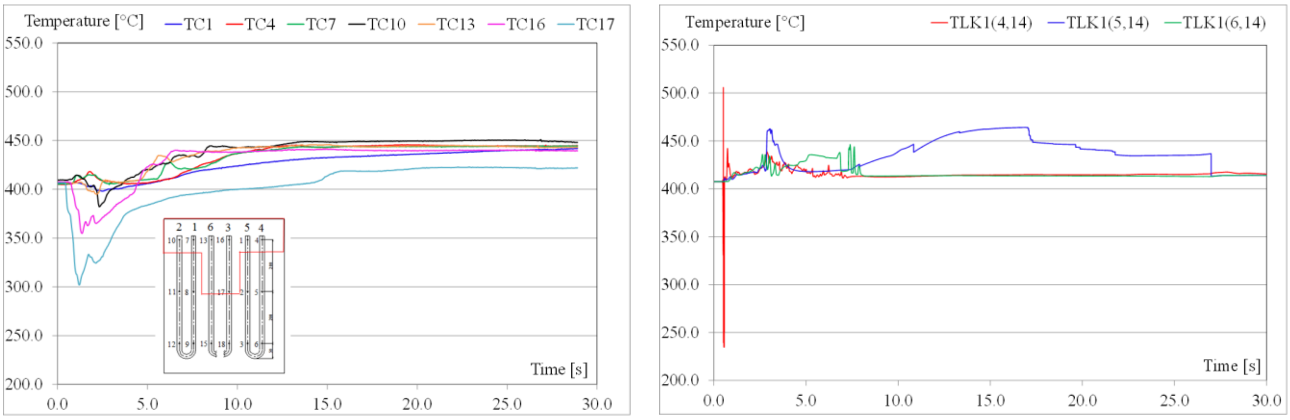

Fig. 4. T#8: PbLi temperature trends in S1. Experimental data (left) and numerical results TLK1 (right).

Table 1. LIFUS5 Test# operating conditions.

Parameter	Test #3	Test#4	Test#5	Test#6	Test#7	Test#8
PbLi temperature [°C]	330	330	330	330	330	430
Water injection pressure [bar]	155	155	150	160	160	160
Water temperature [°C]	295	325	265	320	320	320
Sub-cooling [°C]	50	20	77	27	27	27
Free volume in S5(+S1) [l]	5	5	4	10(+7.5)	10(+7.5)	10(+7.5)
Time of injection [s]	6	6	12	12	12	12

Table 2. Quantitative accuracy evaluation results.

#	Parameter	EXP-CALC	DEV2$_{SIGN}$	DEV2$_{ABS}$	DEV2$_{RMS}$	AA	WF
T#3	Pressure S1	PT5-PK[6,8]	15.15	15.24	17.25	0.21	8.34
	Pressure S5	PT1-PK[6,54]	14.71	14.94	17.76	0.28	9.49
T#4	Pressure S1	PT5-PK[6,7]	8.38	11.60	15.20	0.35	14.39
	Pressure S5	PT1-PK[5,47]	12.82	12.86	18.72	0.57	12.29
T#5	Pressure S1	PT5-PK[6,7]	7.32	9.79	12.48	0.30	9.82
	Pressure S5	PT1-PK[5,47]	6.09	6.99	0.02	0.32	17.57
T#6	Pressure S1	PT5-PK[6,7]	14.62	14.82	15.85	0.16	10.58
	Pressure S5	PT1-PK[5,47]	70.43	70.43	77.03	0.97	8.22
T#7	Pressure S1	PT5-PK[6,7]	13.10	13.19	14.27	0.15	10.97
	Pressure S5	PT1-PK[5,47]	15.34	15.34	21.70	0.27	4.28
T#8	Pressure S1	PT5-PK[6,7]	14.23	14.23	15.03	0.15	9.00
	Pressure S5	PT1-PK[5,47]	10.44	10.49	11.43	0.13	9.01

5. Conclusions

The validation of the SIMMER code for fusion application was conducted against all available data of LIFUS5 experimental tests and applying a standard methodology, commonly used in system code validation. The methodology is based on a three-steps procedure and through qualitative and quantitative accuracy evaluations. The analysis of the results bring the following:

- The modified version of SIMMER-III code for fusion application is able to predict the relevant thermal-hydraulic phenomena during PbLi/water interaction (i.e. pressure trends due to water flashing and evaporation and due to hydrogen generation);
- The temperature trends evidence that the exothermic chemical reaction between PbLi and water is reasonably simulated, although the chemical energy is derived from the TC measurements;
- The correct knowledge of initial and boundary conditions largely affects the SIMMER code results, as well as geometrical features and jet-fragmentation modeling.

The code has demonstrated promising capability in predicting phenomena connected with PbLi/water interaction. The code validation activity is ongoing, and will be conducted applying the methodology once qualified data (i.e. pressures, temperatures, amount of injected water, and hydrogen production quantification) will be provided by next LIFUS5/Mod3 campaign, executed with controlled and well-known initial and boundary conditions.

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