**SIMMER CODES POST-TEST VALIDATION ACTIVITY BASED ON LIFUS5/MOD3 EXPERIMENTS FOR PBLI-WATER INTERACTION**

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Abstract – *The in box-LOCA (Loss of Coolant Accident) is a key safety concern to be addressed in the design of the WCLL-BB (Water-Cooled Lead-Lithium Breeding Blanket). In this accident, a rupture of the tubes in the coolant circuit would cause a severe exothermic chemical reaction occurring between the primary coolant (water) and the Lead-Lithium alloy. The experimental facility LIFUS5/Mod3 was realized at ENEA Brasimone RC to investigate the phenomena associated with the interaction between lithium-lead and water. One of the main objectives of the experimental campaign is to provide data to develop and validate the SIMMER codes to be used on fusion scenarios related to the WCLL-BB safety design.*

*In the present work, post-test numerical simulations carried out by the University of Pisa with the codes SIMMER-III and SIMMER-IV are analyzed and compared against new experimental data obtained in the LIFUS5/Mod3 experimental campaign. It is shown that the code is capable of correctly capturing the main phenomena involved in the experiments, even though the quantitative predictions are still not satisfactory; however, the quantitative results presented and analyzed here are a crucial asset for the ongoing development and validation of the chemical model and are used to address the further steps needed to fully validate the codes.*

**Keywords:** DEMO reactor; In-box LOCA; LIFUS5/Mod3; SIMMER code; WCLL-BB

I. Introduction

The Water Cooled Lithium Lead blanket concept [1]-[2] employs sub-cooled water flowing through the cooling tubes at high pressure, removing heat from the high temperature PbLi eutectic alloy maintained at atmospheric pressure. Although the cooling tubes of reference WCLL blanket design for DEMO are double wall, the probability of lithium-lead/water interaction is still not negligible.

Research activities are ongoing to master phenomena and processes occurring during the postulated in-box LOCA, to address the safety response of WCLL BB system, to enhance the predictive capability of numerical tools, and to validate computer models, codes and procedures for their applications [3 - 9]. Besides, the reliability of qualified system code for deterministic safety analysis is of primary importance, in view of the evaluation of accidental consequences and mitigating countermeasures. Current status of knowledge requires experimental data to support these activities. Nevertheless, the separate effect experiments executed in the past are few and not designed to perform validation activity of DSA code [10]. In view of this, the new separate effect test facility LIFUS5/Mod3 [9] has been commissioned and the Series D experimental campaign has been designed and completed [8-9]. The tests are focused on the generation of experimental data for the validation of the modified version SIMMER codes for fusion application, and numerical simulation activities are ongoing [5 – 11], performed with the modified version of SIMMER-III and SIMMER-IV code, which implement the PbLi/water chemical reaction [11].

The objective of this work is to present a comparison against experimental data of the results of the simulation of one test of the Series D experimental campaign, so called Test D5.1, carried out with the two main versions of the SIMMER code (namely SIMMER-III and SIMMER-IV codes).

II. EXPERIMENTAL CAMPAIGN ON LIFUS5/MOD3 FACILITY

***II.A. Facility description***

LIFUS5/Mod3 is a separate effect test facility that derives from the modification of an existing facility, namely LIFUS5/Mod2, with a new smaller reaction vessel (S1B) [5, 6, 9, 12]. The “section B” of the facility applies the S1B vessel and will be used in the framework of EUROfusion program, to investigate the PbLi-water interaction, Fig. 1. The main objectives of LIFUS5/Mod3 experimental campaign can be explained as the investigation of the relevant physical and chemical phenomena between lead-lithium eutectic alloy and water, and the validation of the chemical model of the SIMMER-III and SIMMER-IV codes. Additionally, the expected outcomes of the experiments are listed below:

•The generation of a detailed and reliable experimental database;

•The improvement of the knowledge of thermodynamic and chemical behavior of the PbLi eutectic alloy;

•The investigation of the chemical reaction evolution and hydrogen production.

***II.B. Test execution***

The initial test conditions were achieved accordingly to the design specifications, a detailed explanation of the experimental procedure, the test matrix for Series D and the main parameters characterizing the tests are reported in [9, 12]. The water injection is started by opening the valve VP-SBL-06 and ended by its closure, which was automatically activated after 1 s, therefore, the injection into S1B lasted 1.1 s (from the injector cap rupture to VP-SBL-06 fully closed). The amount of water injected in S1B was pre-defined as 50 g. The Test D3.1 transient was divided into 3 main phases:

•Phase 1: Injection line pressurization, recorded by PT-SBL-02;

•Phase 2a: Coolant flashing and reaction vessel pressurization, from the injection cap rupture up to the onset of the first pressure peak in the S1B reaction vessel;

o Phase 2b: Pressurization due to the water and gas injections and to the hydrogen generation;

o Phase 2c: Characterized by the continuous gas injection, up to the pressure stabilization;

•Phase 3: System stabilization, from the valve closing signal up to the end of the transient.

III. SIMMER NUMERICAL MODEL DESCRIPTION FOR LIFUS5/MOD3 SERIES D TESTS

Based on LIFUS5/Mod3 facility configuration, the models were developed by SIMMER code Ver. 3F Mod. 01 to support the experimental campaign as a reference model. The nodalizations aim to model both physical and chemical reactions between liquid PbLi and water.

***III.A. Reference LIFUS5/Mod3 Nodalization for SIMMER-III and SIMMER-IV codes***

Considering the geometrical limitation of SIMMER-III code for 3 dimensional purposes, which means it is possible to use solely cylindrical coordinates to fit 3D volumes, the developed SIMMER-III nodalization uses a cylindrical geometry to model the reaction vessel S1B, injection line and the connecting parts. The reaction vessel S1B, the injection line, thermocouples’ supporting passage, hydrogen extraction line, expansion line, are all included in this model as halved symmetric volumes. Rotating the whole volume around the central Z axis in 2D-(R-Z) coordinates gives all volumes and integrated shape of the facility in 3D coordinates. Otherwise, the SIMMER-IV developed nodalization uses a 3D domain to model the reaction vessel S1B, injection line and the connecting parts. The reaction vessel S1B, the injection line, thermocouples’ supporting passage, H2 extraction line, part of the expansion line, are all included in this model as independent volumes.

After the information obtained about the LIFUS5/Mod3 facility in Series D Tests configuration [12], the nodalization was kept fixed, also for all sensitivity analyses, and the final nodalization is described in the following. As it is briefly explained before, because of asymmetric parts of the facility, a set of assumptions was made to simulate the asymmetric layout.

The facility set up for the reference model calculation is shown in Fig. 1. It is constituted by 5 main parts:

•The injection line (all valves, SBL pressurized water pipe and the injector cap).

•The reaction vessel S1B (including Test-Section).

•The expansion line (including the first rupture disk).

•Hydrogen extraction line (up to the collecting valve).

•Thermocouple supporting passage (gooseneck);

The SIMMER-III geometrical domain is obtained by 50 radial and 100 axial mesh cells (Fig. 2) and the SIMMER-IV geometrical domain is obtained by 31\*31 planar and 100 axial mesh cells (Fig. 3 to Fig. 5). Colors distinguish the different fluids and structure material, as set at the beginning of the transient (t = 0 s). Therefore, the PbLi is represented in red, the water in blue, the Argon cover gas (and the hydrogen produced by the reaction) in white, the non-calculation zones are highlighted by green mesh fence and SS316 in black as the structural material. As explained, the overall volume of the model is obtained by rotating the 2D SIMMER domain along the axis of symmetry. The reference mesh cells for the temperature analysis inside the S1B, representing the position of installed TCs in S1B, are highlighted in yellow (see Fig. 2 and Fig. 3). The reference cells for the pressure measuring are also highlighted in purple (Fig. 2 and Fig. 3).

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*Fig. 1.* *LIFUS5/Mod3 configuration, to be used for the SIMMER-III and IV reference model.*

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*Fig. 2.* *SIMMER-III 2D nodalization for LIFUS5/Mod3 Series D campaign.*

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*Fig. 3.* *SIMMER-IV 3D nodalization for LIFUS5/Mod3 Test Series D (IJ plane, K = 16).*

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*Fig. 4.* *SIMMER-IV 3D nodalization for LIFUS5/Mod3 Series D campaign D (IK plane, J = 6, 27, 31,48).*



*Fig. 5. SIMMER-IV 3D nodalization, three-dimensional view and real scale*

IV. Results

The qualitative accuracy evaluation, discussed hereafter, is based on the identification of phenomenological windows associated with the experimental tests [5, 12]. It essentially derives from a visual observation of the experimental and predicted trends. The experimental initial conditions for Test D3.1, together with the numerical ones, are reported in Tab. I.

The calculation transient, during the injection, can be divided into the similar phenomenological windows discussed in [5,12] and summarized as below:

Phase 1 [from SoT to 55.5 ms]: water injection line pressurization. As soon as the valve VP-SBL-06 opens, water starts to flow and to pressurize the pipeline upstream the injection cap. The start of the transient (t = 0 s) is selected as the time of the valve opening (see from Fig. 6 to 11). At the same time, the pressurized water starts to move up and mix with Argon gas. As explained, in Test D3.1, 50 g of water is charged into the injection line and there is not a continuous flow passing through the measuring cell (3,40) for SIMMER-III and (16,16,23) for SIMMER-IV, therefore, there is not a direct way to understand the exact thermodynamic condition of water in the injection line and the only way is to rely on acquired data from TC-SBL-05 and PT-SBL-02. The pressure evolution during Phase (1), proves that the code acceptably predicts the pressurization phase with a small overestimation of first peak in the injection line, see Fig. 6 for S-III and Fig. 7 for S-IV.

Phase 2 [from 55.5 ms to 1158 ms]: water and gas mixture flashing into S1B and the vessel pressurization followed by PbLi/water reaction. This phase can be further divided into three sub-phases:

(2a): Coolant water flashing and first pressure peak. The water injection and flashing in the liquid metal inside the reaction vessel causes a sudden steep pressure peak. The peak is high but also unstable, and it reaches to 25 bar at cell (50,56) in SIMMER-III calculation and 22 bar at cell (31,16,34) in SIMMER-IV calculation, while the relevant recorded values for PT-S1B-01/02/03 range between 35-46 bar for Test D3.1. In the following, the pressure decreases slightly for a very short period, which is immediately followed by the next arising peaks, see Fig 8 and Fig. 9. The calculation reports more peaks at the very beginning of the flashing phase, but these peaks are disappeared faster comparing to the experimental signal. The pressurization signal in the injection line is closely reproduced by the numerical model for PT-SBL-02. The first peak value at PT-SBL-02 in the experiment is 143 bar while it is 148 bar in the S-III reference calculation and 143.6 bar in the S-IV calculation.

(2b): Pressurization due to water and gas injection and hydrogen generation, characterized by the water injection and hydrogen production. The pressure and temperature trends show the PbLi/Water interaction inside S1B, the influence of this interaction is measured and plotted against the same relevant experimental data at the Test Section, see from Fig. 6 to Fig. 11. Almost all hydrogen is produced in this sub-phase through the chemical reaction between the liquid PbLi alloy and water in both vapor and liquid phasesas shown in Fig. 12 and 13.

Nevertheless, in general, the trends give a similar phenomenological notion as for the performed experiment, by stating that the interaction impact on temperature is higher and earlier in time along both radial and axial directions. In other words, it means that the closer cells to the injector cap take more influence from PbLi/Water interaction while this impact becomes lower and delayed in time for outer cells. In this phase, all the injected water is exhausted through the chemical reaction with PbLi

(2c): characterized by the continuous gas injection up to the pressure equilibrium. During this sub-phase, the pressure measured by PTs in S1B show a very linear increase inclining towards the final equilibrium pressure. In this phase, the most dominating effect is the Argon gas pressure at the boundary cell (50,19) and (16,16,1), see Fig.10 and Fig. 11.

Phase 3 [from 1158 ms to EoT]: system pressure stabilization, from valve closing signal to the EoT, transient ending stage. This phase is characterized by the stabilization of pressure and temperature in the system, which is immediately, started by shutting off all the valves. This is to isolate S1B and prevent from either extra Argon gas injection or reverse flowing of the liquid PbLi into the injection line and defecting the fast actuation valves. During this phase, the injection valve is closed, and the parameters are stabilized (Fig.10 and Fig. 11).

From a qualitative analysis of the transient, SIMMER codes reasonably predict the pressure trends. The final pressures in S1B stabilize in the simulation at 91 bar and between 87 and 89 bar (@ PT-S1B-01/03) in the experiment.

The hydrogen production trend due to the chemical reaction and estimated by the codes is shown in Fig. 12 and 13, and the final value (once all the water is consumed) is equal to 3.9 g (S-III) and 2.8 g (S-IV) at the end of Phase (2). In the experimental test D3.1 the hydrogen was recorded and reported equal to 1.93 g, but the stoichiometric calculation gives 2.7 g and 5.5 g, based on the two parallel chemical reactions (on producing Li2O as product and the other one producing LiOH).

*Table I Initial conditions: Experiment and simulations*



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*Fig. 6. Pressure (PK) in S1B and imposed BC position compared with experimental data (PT), Focus on [0.03-0.08 s] – SIMMER III calculation*

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*Fig. 7. Pressure (PK) in S1B and imposed BC position compared with experimental data (PT), Focus on [0.03-0.08 s] – SIMMER IV calculation*

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*Fig. 8. Pressure (PK) in S1B and imposed BC position compared with experimental data (PT), Focus on [0-0.5 s] – SIMMER III calculation*

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*Fig. 9. Pressure (PK) in S1B and imposed BC position compared with experimental data (PT), Focus on [0-0.5 s] – SIMMER IV calculation*

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*Fig. 10. Pressure (PK) in S1B and imposed BC position compared with experimental data (PT), Full transient [0 – 1.5 s] – SIMMER III calculation*

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*Fig. 11. Pressure (PK) in S1B and imposed BC position compared with experimental data (PT), Full transient [0 – 1.5 s] – SIMMER IV calculation*

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*Fig. 12. Total mass of produced hydrogen - SIMMER III calculation*

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*Fig. 13. Total mass of produced hydrogen - SIMMER III calculation*

V. Conclusions

This paper presents part of the results carried out for the validation of SIMMER-III and SIMMER IV codes, which are under development at the University of Pisa to be extended towards fusion application, through the comparison with experimental data obtained with the LIFUS5/Mod.3 during the Series D tests of the experimental campaign. The main focus in the analysis of the results discussed here concerns the pressurization of the injection line and the pressurization of the S1B vessel, together with the proper estimation of the hydrogen generation due to the chemical interaction between lead-lithium and water.

Based on the experimental data, the code predicts the pressure of injection line during the line pressurization in Phase 1. During Phase 2a, the code captures and predicts the first pressure peak due to the injector cap break-up and water flashing into S1B. However, both SIII and SIV slightly underpredict the peak value. The pressure trend is qualitatively in line with the experimental results, even though the pressure increase rate in the injection line is never exactly matched. Some differences occur during Phases 2b and 2c, indeed the code calculates an anticipated onset of S1B pressurization. Furthermore, from a quantitative point of view, the pressure inside the S1B and the injection line during these two subphases is always overpredicted with an offset of 5-10 bar, with the values getting closer to the BC than to the experimental data. The behavior is affected by the fragmentation and continuous injection of argon, but the experimental signals are reproduced in both the injection line and S1B.

The codes results are promising also during Phase 3. The final difference between the reference calculations and the experiments remains less than 10-15 bar for all the cases. The code results are significantly aligned with the experimental trends, however, the overprediction of the pressure seen in phases 2b and 2c remains also in this phase, especially for SIMMERIV. The reasons of this overprediction might require further investigation.

Furthermore, the numerical results for the hydrogen generation seem acceptable and coherent with the experimental results and the stoichiometric calculation.

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