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№ 9711

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February 14, 2023

Proceedings of the 9th International and 49th National Conference on Fluid Mechanics and Fluid Power (FMFP)
December 14-16, 2022, IIT Roorkee, Roorkee-247667, Uttarakhand, India

FMFP2022–6535

Numerical investigation of LIFUS5/Mod3 Series E Experiment Test 5.1 towards thermal-hydraulic system code SIMMER-III validation

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ABSTRACT

Under this study, the LIFUS5/Mod3 series E experiment Test 5.1 is being numerically investigated and compared with the experimental parameters to validate the thermal-hydraulic safety analysis system code "SIMMER-III" for the interaction of lead-lithium and water under circumstances like those anticipated for the Water-Cooled Lead Lithium Breeding Blanket (WCLL BB) under accident situations so that the code can accurately predict these transients and accidents. Experimental studies continue to be conducted to investigate the dynamics and reactions that occur during a hypothesized in-box LOCA in the WCLL BB and throughout the system's protective response by the University of Pisa and ENEA Brasimone Research Center. Additionally, several initiatives are being undertaken to enhance the predictability of computational tools and validate the safety analysis system codes, modeling techniques, and successful implementation.
In particular, the experimental Test E5.1, conducted in the distinct effect test facility LIFUS5/Mod3, has been numerically reproduced for the present study (installed at ENEA Brasimone Research Center). The University of Pisa updated a version of the SIMMER-III numerical algorithm utilized for the mathematical model to accommodate the chemical interaction between the two fluids.

Keywords: Multi-Phase flow, SIMMER-III system code, Lead-Lithium, and water interaction, LIFUS5/Mod3 facility, code Validation.

1. INTRODUCTION

For the European DEMO nuclear fusion power plant, water-cooled lithium-lead (WCLL) BB is a viable alternative that has lately been taken into consideration [1-2] in addition to the TBM initiative [3]. The high-pressure, sub-cooled water used in the WCLL blanket idea transfers the heat from the high-temperature lead-lithium eutectic while keeping the fluid pressure constant about 1 atmosphere. The benchmark WCLL blanket design's coolant channels are double walled, yet the likelihood of lithium-lead/water encounter owing to a hypothesized in-box LOCA is nevertheless significant. The introduction of water into a liquid metal reflects both a direct exothermic reaction that raises both pressure and temperature because of combined thermal and chemical reactions and an indirect energy release those results in the formation of hydrogen because of subsequent chemical oxidation the byproducts of the immediate reaction. The conceptual framework of the WCLL blanket is affected by the issue of determining whether this interaction caused by a water leak into the PbLi can break the blanket enclosure or if this hazard can be eliminated altogether.

2. LITERATURE REVIEW AND OBJECTIVE

Studies are being done to learn more about the behaviours and mechanisms that happen in most of the hypothesized in-box LOCA, to figure out how sensitively the WCLL BB system needs to be protected, to improve the ability of computational tools to predict, and to test simulation techniques, algorithms, and methods for their use. Also, the accuracy of the certified nuclear thermal-hydraulic safety analysis system code for predictive safety analysis is vital for figuring out how accidents might happen and producing ways to stop or lessen their effects. Measured results are needed to back up these efforts, considering the current state of research. However, the few special effects tests conducted in the past were not intended to conduct DSA coding verification and validation [4-5]. Considering this, the Series E experimentation program is underway, and the new separate effect test facility LIFUS5/Mod3 [5] has been established. The main goal of the experiments is to get scientific data that can be used to test and confirm the SIMMER code variants used in fusion applications. As part of the Evaluation and Validation activity [4-5], methods must be standardized using measured results with well-defined and repeatable starting and operating conditions. The updated SIMMER-III algorithm has models [6] that use the chemical reaction between PbLi and water [7]. The results of the experiments will also help with the new tool for calculating STH/2D coupling.
Additionally, information will be utilized to investigate the interactive impacts of energy output on the components and to generate pertinent input for the repeated measurement sessions. The primary goal of this work is to verify the thermal-hydraulic safety analysis system code "SIMMER-III" for the interaction of lead-lithium and water in conditions comparable to those expected for the Water-Cooled Lead Lithium Breeding Blanket (WCLL BB) under accident scenarios by numerically investigating and comparing it with the experimental parameters. The University of Pisa's Department of Civil and Industrial Engineering's Laboratory of Numerical Simulations

for Nuclear Thermal-Hydraulics and the ENEA Brasimone Research Centre are continuing their experiments to study the dynamics and responses that happen in the WCLL BB during a hypothetical in-box LOCA and during the system's defensive response. Additionally, some activities are being conducted to improve the predictability of computational tools and evaluate the codes, modelling methods, and effective implementation of safety analysis systems.

3. MATERIALS AND METHODS

The LIFUS5/Mod3 experimental facility is an upgrade from LIFUS5/Mod2 to support the brand-new series D and E experimental campaigns. The S1A, the water storage tank (SBL), the expansion container (S3V), and the current reaction vessel are all still in service. A modest reaction vessel (S1B) has been installed in accordance with the PED guidelines and is suitable for usage at pressures and temperatures up to 200 bars and 500°C. In the event of a rupture disk activation, the S3V dump vessel, which is shared by both sections of the facility, is utilized to collect cover gas or other compounds discharged from the interaction vessels. The component B of the facility, which is dedicated to the EURO fusion consortium and utilizes the S1B reaction vessel for PbLi/Water interaction research, is exclusively included in the following description. The primary reaction vessel (S1B), in which the interaction between liquid lead-lithium and water occurs, is one of the five main parts of the facility. The other four are the injection line, which connects the bottom of SBL to the bottom of S1B, and the SBL cylinder, which is used to store and transport water to the experimental conditions. In order to protect the experimental setup in the event of overpressure, emergency expansion tank S3V is connected to S1B with two rupture plates; S4B1 and S4B2 lead-lithium storage vessels for pure and used alloy; and an argon cylinder attached to the top of the SBL maintain pressure all across the period of injection.

The LIFUS5/Mod3-section B facility is described in depth and the key components of facility are listed in the literature [4]. The LIFUS5/Mod3 experimental facility has been altered, and the Series-E experimental campaign has been intended to model and accurately simulate the LOCA incident through the break in the water tank up to the absolute balance between the water channel and the BB box to examine these processes, linked to the protection of the WCLL BB configuration. Figure 1 shows the synoptic of LIFUS5/Mod3 experimental facility while performing the test E 5.1.

3.1 Test E5.1

The findings of the E5.1 Test, which was performed on November 18th, 2020, utilizing the experimental apparatus LIFUS5/Mod3 of CR Brasimone (ENEA), are undertaken throughout this publication. In fact, it can deliver: 1) all the experimental data collected by the sensor module that is readily accessible; 2) results appropriate to the test boundary and initial conditions; 3) a subsequent study and processing of the findings, and 4) the data necessary for a more in-depth evaluation and implementation of the post-test evaluation employing numerical codes.

The experiment investigates the safety of breeding blanket in the water. The primary goal of the experiment is to gather authentic and thorough data sources for evaluating and validating the chemical model used in SIMMER-III ver. 3F Mod0.1, enhancing our knowledge of the reaction between lead-lithium and water. At 176.5 bars and 264.2ºC, water was introduced into reaction vessel S1B, which contained lead-lithium eutectic. The experimental examination looks at how pressure and temperature transients change over time, as well as the evolution of the hydrogen created by the chemical process between the two substances. The chemical stimulation of the lead-lithium-water interaction created by the SIMMER software will be validated using these data. Table 1 lists the various parameters, operating conditions, and SIMMER-III inputs that were created during the execution of the experiment.

3.2 Code model

The lead-lithium and water thermo-chemical models were included in "SIMMER-III Ver. 3F Mod. 0.1" [6], an enhanced version of the code developed at the University of Pisa, Laboratory of Numerical Simulations for Nuclear Thermal-Hydraulics Department of Civil and Industrial Engineering [4]. The main objectives of post-test simulations are validation and verification of the current chemical model in the code version, investigation of modifications required in the code model based on post-analysis and experimental results, and comparison to replicate the experimental results more precisely numerically under various scenarios.

Following the analysis of the experiment test E5.1, different numerical calculations are simulated for a range of orifice discharge coefficients and lead-lithium-water reaction rate coefficients, which are very versatile and heavily reliant on the thermal-hydraulic conditions of the system, fluid dynamic regulatory frameworks, and scheme configuration [8]. The outcomes of this step confirm and verify the SIMMER program, particularly for the specific circumstances used in Investigation Test 5.1. A reference input for the LIFUS5/MOD3 SIMMER-III simulation analysis, utilized as the beginning and operating conditions, is shown in Tab. 1, together with the composite test information as well as other input circumstances of investigation test E5.1. The system's geometrical nodalization consists of 50 radial and 100 axial cells in cylindrical coordinates (see Fig. 2).

In two-phase control volumes in the grid with a tiny void percentage, the vapour temperature was changed to prevent instability in the numerical calculations. The molecular momentum diffusion and turbulence-diffusion terms are specified in all relevant indicators. Since the SIMMER-III algorithm only calculates resistance in the mesh cells, including the "can wall" structures, the injector line friction was disregarded in the chemical reaction calculation process. The localized pressure decreases due to the geometric mean at the injection device's aperture. To contain the optimum value, the input file's orifice coefficient of adjustments and curvatures are drawn using empirical equations, but because they are sensitive, an utterly separate assessment is also carried out to determine their accurate value.

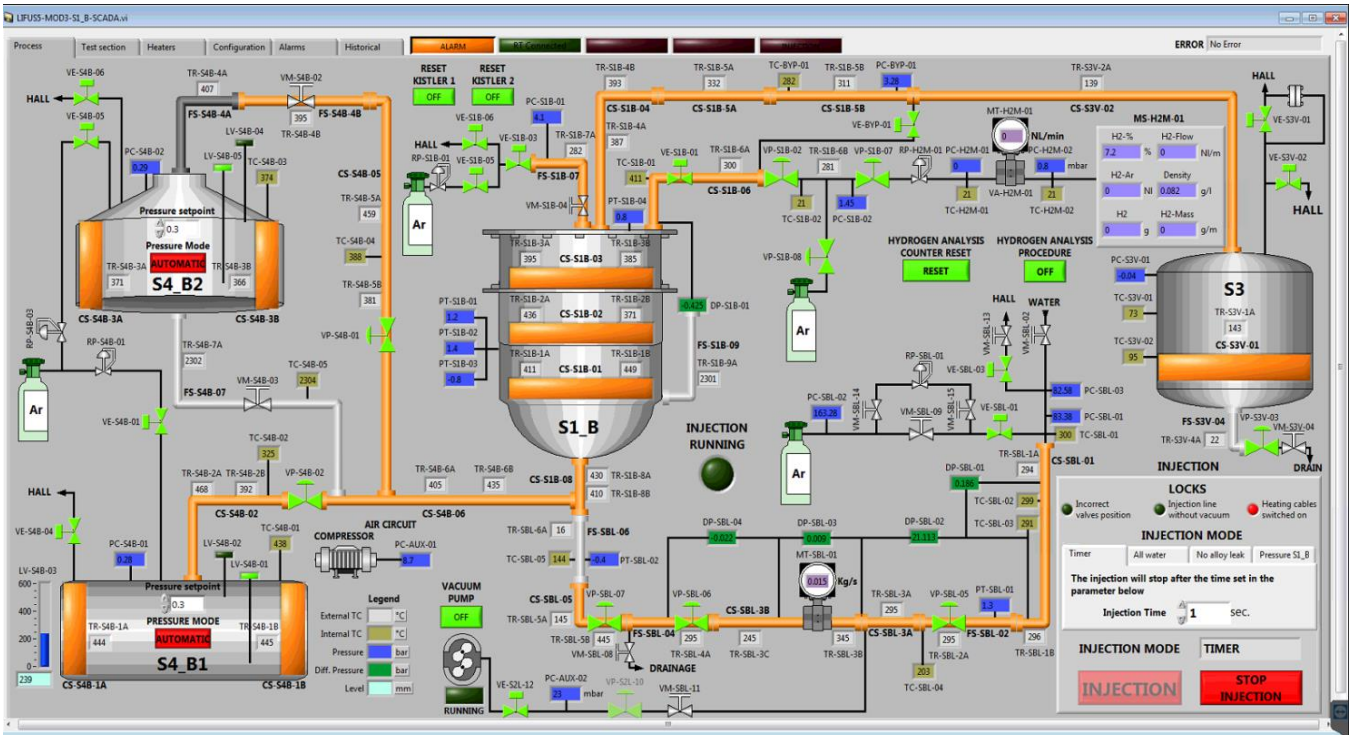

Figure 1: **LIFUS5/Mod3 facility, synoptic**

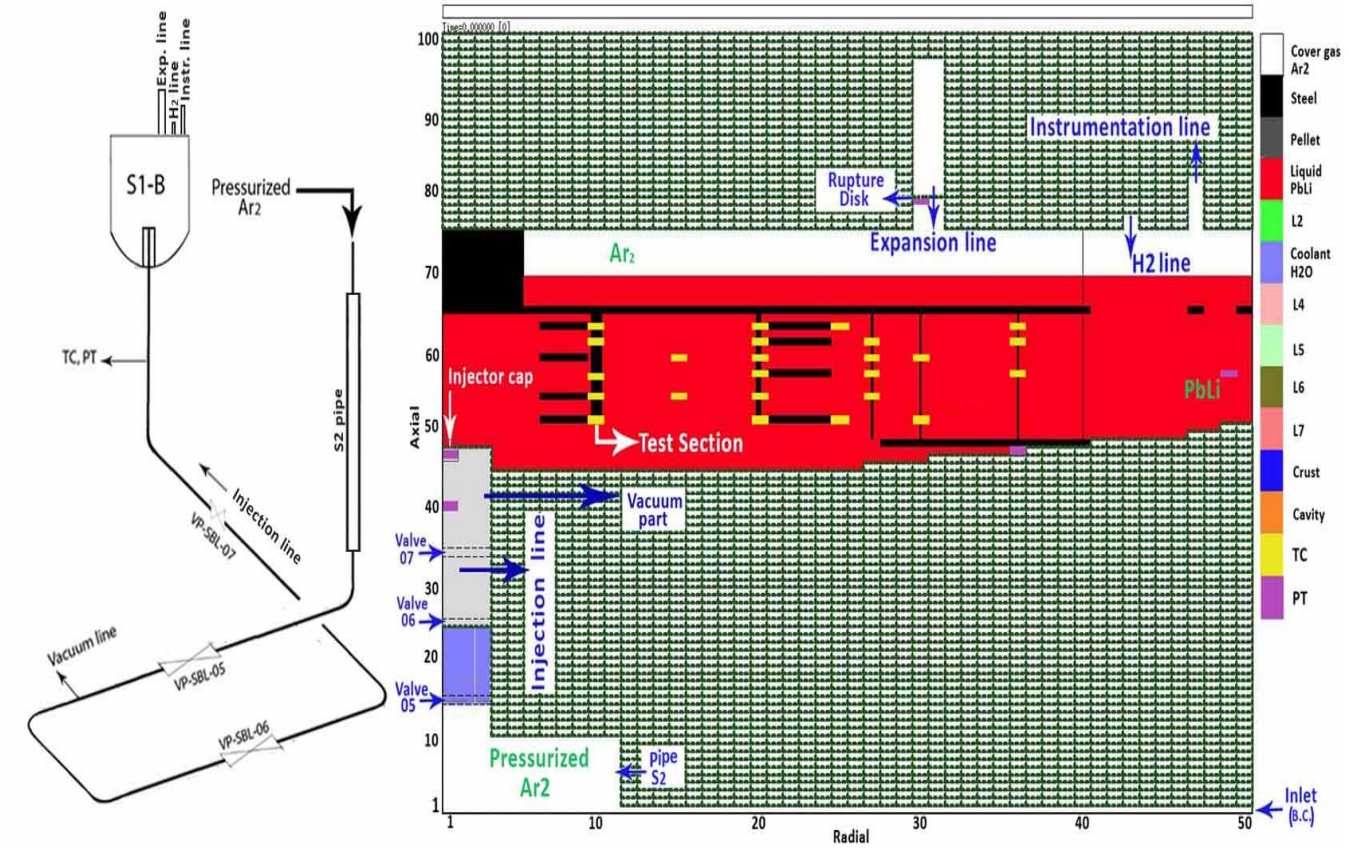

Figure 2: Thermal-hydraulic nodalization SIMMER-III, injection line (SBL), and reaction vessel (S1B) for LIFUS5/Mod3

Table 1: LIFUS5/Mod3 Test 5.1 input boundary conditions

#	Test E5.1			
	Parameter	Design	Actual	SIMMER-III
S1-1	P @ SoT (bar)	1	0.24	0.24
S1-2	T_{PbLi} @ SoT (°C)	330	324.2	324.2
S2-2	P @ SoT (bar)	155	176.5	176.5
S2-3	T @ SoT (°C)	295	264.2	264.2
S2-7	Water-injected (g)	--	198-259	280-300
I-2	Injection on (s)	0	0	0
I-3	Injection time (s)	1.5	1.4422	1.4422
I-4	Injector cap rupture instant (s)	--	0.2219	0.2219
I-7	Injection valve fully closed (s)	1.5	1.476	1.476
I-8	Nozzle orifice (mm)	1	1	1
I-9	Injector length (mm)	20	20	20

4. ANALYSIS AND RESULTS

The LIFUS5/MOD3, Test 5.1, post-test simulation using the stand-alone SIMMER-III system code has been performed successfully and compared with the experimental data. By comparing the optimized outcomes of the code with experimental data, we may conclude that the code can simulate the situation produced by Test Circumstances E5.1. This test simulation ensures that the code is providing accurate results as compared to the experimental data and works in different thermal-hydraulic and system environments. For the simulation to work, the reference input file was created according to the parameters listed in Table 1. The boundary and input conditions were taken from Table 1. The experimental data were used to determine the input variables (temperature and pressure) of the thermal-hydraulic model that depends on time. In the previous sections (SIMMER-III code model), we talked about the simulation parameters, correlations for different thermodynamic and heat flow dynamics, the framework of direct interaction between lead-lithium and water, and the equation of state framework that was considered for the study. The key conclusions from the simulation studies of test E5.1 are examined and presented in this section. The experimental and simulated transients have four main observational phases that are different from each other that split into three stages based on their characteristics. Figures 3 and 4 show the related dynamical patterns and the order of events that happened during the post-test and the experiment.

Phase 1: The water injection line is pressurized (0–221 ms from when the valve opens to when the injector cap breaks). When the VP-SBL-06 valve is opened, water starts to flow and pressurize the upstream pipeline. The valve opening time is the transient's beginning (t = 0 s). Based on the results of experiments, time-dependent pressure conditions are set at the top of the injection line to simulate the flow of Argon gas from the cylinder through the line; see node (50,1) in Fig. 2. The cap rupture instance is chosen for the simulation using experimental data, around 36 ms after the SOT. The removal of a virtual wall at the top of the cell simulates the cap rupture (1,47). Figure 3 depicts the pressurization trend of the injection line throughout this period.

Phase 2: Water-PbLi reaction [221 ms to 1664 ms (EoI)], from cap rupture to completely closed valve VP-SBL-06. This process can be separated into three comment sections: 2(a) Injected water flashing [221 ms to 300 ms] from cap breach to the last stage of the first pressure spike,

2(b) from the end of the early pressure peaks to the change in the pressure slope [300 ms to 510 ms], thermodynamic effects cause the pressure to rise, and

2(c) from pressure curve change to entirely closed valve VP-SBL-06, chemical reaction predominates pressurization [510 ms to 1664.1 ms] (EoI). The pressure spike reaches 2.1 bar in the reaction vessel's S1B zone's reference cells (50, 56) (Fig. 3(a)). The pressure gradually decreases afterward. As soon as the orifice breaks, the pressure of the displacing fluid immediately increases; however, as the shockwave spreads across the reaction vessel, the pressure drops (pressure peak is absorbed quickly due to the large compressibility of cover gas Argon above the PbLi region). The anticipated mass flow rate of the injected water (Fig. 3(b)) increases concurrently with the pressure peak and subsequently decreases due to increasing pressurization in the reaction chamber. Figures 3(a) and 3(b) (SIMMER-III computed and experimental) depict the absolute pressure and flow rate patterns. In the whole transient, there was excellent agreement between what SIMMER-III anticipated and experimental results, as shown in Fig. 3. Notwithstanding, water continues to be injected continuously until the phase has been completed (1.476 s), after which the pressurization of S1B causes the flow rate to increase once again and then fall. Although the quantity of hydrogen created during stage 2 is negligible, it increases during the surge and eventually reaches stabilization during stage 3. The computations of the code reveal that phase 2 of the lithium-water reaction mechanism remains negligible. Phase 2 is when the cooling effect of the water has a more significant impact on temperature than the heat produced by the chemical reaction (Fig. 4). Aspects 3b and 3c: Due to the thermodynamic interaction and evaporation, the pressure within S1B gradually rose to around 5 bar, starting at about 300 ms. When valve VP-SBL-06 is shut off, the pressure increases again and climbs to 13 bar. This phase is dominated by the pressurization brought on by the exothermic chemical interaction between PbLi and water, the following hydrogen production, and temperature increase (see the temperature trends in figure 4 inside the S1B reaction vessel). After phase 2, SIMMER-III estimated the total quantity of water injected

into S1B to be about 280-300 g, while the experimental value was approximately 30 g (Fig. 3 (c)). Even though during this phase, about 20-25 g of hydrogen is created (Fig. 3(d)).

Phase 3: From the time the valve VP-SBL-06 is completely closed (EoI) until the initial pressure stabilization, which lasts from 1476 milliseconds to around 2000 milliseconds. The reaction vessel (S1B) was separated from the injection line (SBL) when valve VP-SBL-06 closed (at 1.476 s). However, the broken injection cap still linked the upper part of the injection line to the reaction vessel (S1B), which holds up some remaining water at elevated pressure. As a result, more water is injected into the reaction chamber. As shown in Fig. 3(c), the remaining water that leaks out of the injection line after VP-SBL-06 is fully closed causes more pressure to build up after the injection stops. However, the pressure rise caused by this process is minimal compared to the pressure rise caused by the chemical reaction.

The reaction vessel pressure progressively rose from 8 to 13 bar as the Pb-Li chemically interacted with the remaining water. Reaction vessel temperatures remained constant.

Phase 4: Chemical reaction dominates pressurization (2000 ms–3500 ms). Due to two factors, the pressure inside the S1B reaction vessel kept rising: first, it tended to equalize with the pressure inside the injection line (though this contribution is limited given the injection line's small volume, especially in comparison to the reaction vessel); and second, it was brought on by the chemical reaction. (The most valuable input.) As a result, the reaction zone's temperatures increased considerably once again (see Fig. 4), and hydrogen release helped to increase pressure without significantly changing its pace. Pressure equalization between S1B and the injection line downstream of VP-SBL-06 occurs at approximately t = 6 s because of the early cap rupture. The plateau can only be achieved at EoT, which is not examined in this research due to convergence issues, and stability occurs at a moderate fall. Figure 4 shows that no significant peaks were seen well during injection (when the VP-SBL-06 valve opened), but the global average temperatures showed that the chemical interaction was strongest in the central levels (Levels 3, 4, and 5), but it was also spread out in a lateral direction (from Ring 1 to Ring 4). However, the heat produced by the chemical reaction caused an overall rise in temperature in the entire system with an average value of about 7°C (up to valve closure). The experimental results support the simulated dynamics of the PbLi/water interaction; in fact, the thermodynamic interaction dominates the first hundreds of milliseconds after cap rupture, with a chemical reaction that produces hydrogen and a rise in temperature as the secondary processes.

4.1 Code sensitivity

Due to modelling issues, the highly turbulent nature of governing phenomena, numerical model convergence, and the stability of the underlying conservation equations [9,10], the algorithm sometimes generates noticeably erroneous results. They happen when the flow is very turbulent, when condensation and evaporation are predominant, when there is natural circulation, and when the pressures in the two systems are equal. However, by effectively using fluid dynamics algorithms, time steps, control volume axial and radial length ratio, chemical reaction rate, discharge coefficient, etc., these problems were effectively resolved.

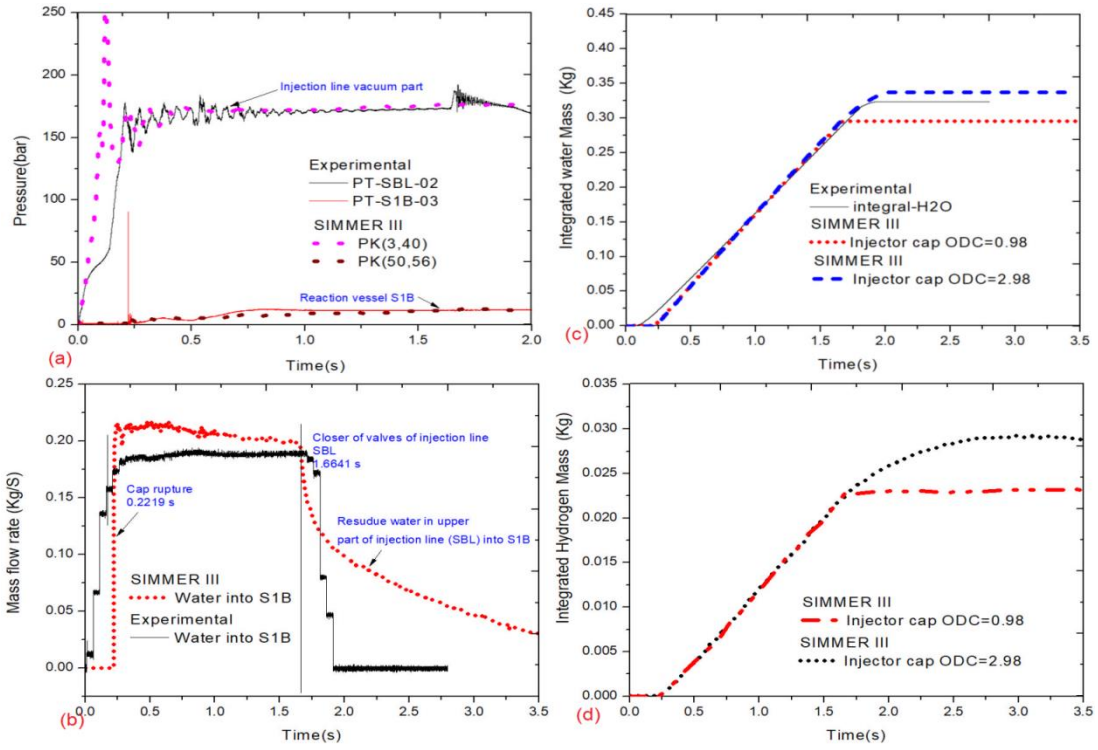

Figure 3(a) trends in pressure in the reaction vessel and injection line; 3(b) the mass flow rate profile; 3(c) the integrated injected water profile; and 3(d) the integrated hydrogen produced during the transient in the reaction vessel.

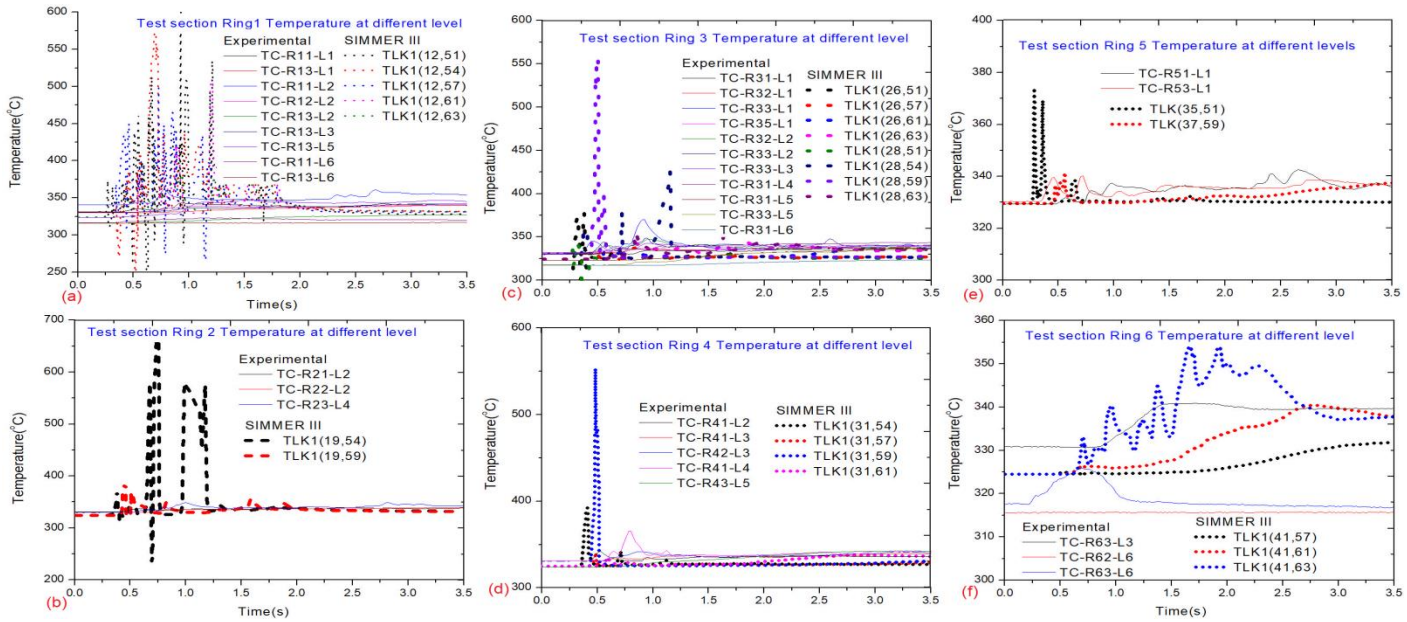

Figure 4: Temperature trends in reaction vessel S1B (a) Ring 1, (b) Ring 2, (c) Ring 3, (d) Ring 4, (e) Ring 5 and (f) Ring 6

5. CONCLUSIONS

Some major findings of the exercise performed in this article are reported below:

1. Utilizing the initial boundary conditions employed during test execution, the simulation of experiment E5.1 by system code SIMMER-III is carried out effectively and validated with experimental information.

2. This publication reports the finest results after several runs of modifying the delicate and unpredictable variables (like orifice discharge coefficient and coefficient of chemical reaction rate).

3. Considerable agreement exists for the critical variables all across the transient between the simulated results and the experimental data (pressure and temperature trends in the reaction vessel). It demonstrates the code's model progressiveness towards predicting thermodynamic and chemical interactions of Pb-LI and water, especially in the context of this specific experimental test E5.1.

ACKNOWLEDGEMENTS

This work has been conducted within the framework of the HORIZON2020, Call H2020-MSCA-IF-2020, funded by the European Research Executive Agency (REA) via the Marie Skłodowska-Curie Actions (Grant Agreement No 101030496). Although all the experimental facilities for the experimental campaign are made available by ENEA Brasimone Research Centre. However, the ideas and thoughts presented are solely those of the author(s) and do not necessarily represent the views or opinions of the European Union or the European Commission. They are not the responsibility of the European Union or the European Commission.

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