

EUROFUSION WPBB-CP(16) 15519

M. Eboli et al.

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Preprint of Paper to be submitted for publication in Proceedings of 29th Symposium on Fusion Technology (SOFT 2016)



This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission. This document is intended for publication in the open literature. It is made available on the clear understanding that it may not be further circulated and extracts or references may not be published prior to publication of the original when applicable, or without the consent of the Publications Officer, EUROfusion Programme Management Unit, Culham Science Centre, Abingdon, Oxon, OX14 3DB, UK or e-mail Publications.Officer@euro-fusion.org

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Consistent Post-Test Analyses of LIFUS5 Experiment

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The interaction between lithium-lead and water is a major concern of Water Cooled Lithium Lead (WCLL) breeding blanket design concept, therefore deterministic safety analysis of the in-box LOCA postulated accident is of primary importance. The paper presents the preliminary code assessment process of the modified version of SIMMER-III code for fusion application by means of LIFUS5 Test#3 post-test analyses. A series of sensitivity calculations are performed to overcome uncertainties in the test data and experiment execution, and to investigate the capability of the code in predicting the phenomena occurring during PbLi/water interaction. Results show agreement between numerical results and experimental data. Besides, differences are observed in the first second of the transient due to imperfect knowledge of initial and boundary conditions, and test execution procedure.

Keywords: water, lithium-lead, SIMMER, chemical reaction, WCLL breeding blanket, safety

1 Introduction

The safety issues connected with the lithiumlead/water interaction in WCLL breeding blanket is a potential hazard that shall be considered. Therefore, the availability of qualified system code for deterministic safety analysis of in-box LOCA accident is of primary importance. The modified version of SIMMER-III code for fusion application, which implements the PbLi/water chemical reaction, has been developed by University of Pisa and ENEA CR Brasimone [1]-[2] and currently is under validation process.

The aim of the paper is to describe the preliminary code assessment of SIMMER-III Ver. F Mod.0.0 code by means of LIFUS5 Test#3 post-test analyses. To address this objective, Section 2 briefly describes the Test#3 experiment, then the nodalization of the facility is reported in Section 3. Post-test analyses results are illustrated in Section 4, in which considerations about the comprehension of experimental data are discussed. Finally, conclusions are reported in the final section.

2 Description of LIFUS5 Test#3

2.1 Facility description

LIFUS5 [3]-[6] was designed and operated at ENEA CR Brasimone to experimentally investigate the consequence of LOCA accidents in liquid metal pools. Fig. 1 shows the P&ID of the facility, descripted in detail in literature [3]-[6]. The reaction vessel S1 contained a mock-up of U shaped cooling tubes, as foreseen in previous design of WCLL BB for DEMO [7]. 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 and thermocouples were placed both in S1 and S5 to follow the pressure and temperature evolution during the interaction.

2.2 Test#3 conditions

Before the execution of the 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 S2 to S1 through the injection line. The water injection pressure was fixed at 155 bar and kept constant through a constant pressurization of the vessel S2. After 6 s, the injection was interrupted closing the valve. The main operating conditions of Test#3 are summarized in Table 1.



Fig. 1. P&ID of LIFUS5 facility

2.3 Open issues

The experimental results described in Ref. [4] are not exhaustive. Moreover, on the basis of the review of available documents, the execution of the experiment is affected by uncertain data in relation to:

- *Thermocouples position* installed in U-tube mock-up, which is not univocally determined, but two different schemes were found in literature (Refs. [3] and [6]).

- *Identification of the injection valve,* because literature reports uncertain information (V14 Refs. [5]-[6] or V4 Ref. [3]).

- *Injected mass of water*, because no mass flow meter was installed in the injection line. In literature, this value was reported as 1.3 kg ([3]-[6]) but no accuracy is reported as well as no reference on the procedure used for the evaluation. This value is considered unreliable.

- Layout of the expansion tubes. No document was found for the configuration of the expansion tubes and a

3" pipe connecting S1 and S5, but only the expansion tubes main dimensions are available (Refs. [3]-[6]).

Tal	ble	1.	Test #:	3	operating	cond	litions.
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Parameter	Test #3
PbLi temperature	330 °C
Water injection pressure	155 bar
Water temperature	295 °C
Sub-cooling	50 °C
Free volume in S5	51
Time of injection	6 s

3 LIFUS5 nodalization by SIMMER-III

The nodalization of LIFUS5 by SIMMER-III Ver. F Mod.0.0 code (the version for fusion application which implements PbLi/water chemical reaction) [1]-[2] is developed in 2D axisymmetric geometry, despite the limitation of representing the asymmetries of LIFUS5 facility. It is constituted by 5 main parts (Fig. 2) representing the water tank S2, the injector device, the reaction vessel S1, the expansion tubes, and the expansion vessel S5. The geometrical domain is obtained by 17 radial and 28 axial mesh cells. Colors distinguish the different fluids, as set at the beginning of the transient: PbLi represented in red, water in blue, cover gas (and the hydrogen produced by the reaction) in white. The overall volume of the model is obtained rotating the 2D SIMMER domain along the axis of symmetry. It is worth to underline that this nodalization considered as first attempt to validate the SIMMER-III code for fusion application is the same of past numerical activities, reported in Refs. [5], [8].



Fig. 2. LIFUS5 facility nodalization by SIMMER-III

The boundary conditions are applied in S2 cover gas cells to reproduce the continuous inflow of Argon from the cylinder, at the constant pressure of 155 bar. The initial conditions of pressure and temperature in S1, S5, and in the injection line, are set coherently with the data reported in Table 1. The reference run is set opening the virtual wall, which represent the valve V14 at t = 0 s, and it is maintained open for 6 seconds, coherently with the experimental specifications. The amount of water injected is not imposed, but calculated by SIMMER-III accordingly to pressure difference between the injector inlet and the reaction vessel.

4 Analysis of Post-test calculation results

Three-step analysis is pursued as a part of the code assessment process. The initial condition results at the injection time are relevant for the characterization of the thermal-hydraulic conditions at the beginning of the experiment. The reference calculation results are achieved from the "qualified" nodalization. It is not the best calculation because is based on a former analysis set-up running the code without the chemical implemented model [5], [8]. Sensitivity analyses 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, to improve the understanding of experimental data, and to improve the knowledge of the code by the user.

4.1 Analysis of code results

The transient can be divided into the three characteristic phases of the interaction [4] plus two additional phases. The numerical and experimental pressure trends are reported in Fig. 3, while Fig. 4 shows the water mass flow rate and the hydrogen generation calculated by the code.

Phase 0 [onset of valve opening -0ms]: water injection line pressurization. As soon as valve V14 opens, water starts to flow and to pressurize the pipeline upstream the injection cap. The design of the test specifies that the cap should be ruptured at the reference pressure (i.e. 15.5 MPa). This implies that subcooled water at 295 °C will enter in S1. During this phase, no measured experimental datum is available. Therefore, according with the set up reference calculation, the start of the transient (t = 0 s) is supposed to be the time of the injection cap breaking. The simulation assumes that subcooled water at the design test conditions is injected directly in the reaction vessel S1.

Phase 1 [0s - 200ms]: coolant flashing and S1 pressurization. The water injection and flashing in S1 causes a sudden steep pressurization. The code results evidence a faster pressure increase. The calculated pressure peak is 12.7 MPa occurring at about 20 ms, whereas the experimental value is 10.0 MPa at 200 ms. Different causes are identified for justifying these trends. However, considering the data of Test#6 [9] where the pressure was measured in the injection line, the most likely justification is an early rupture of the injection cap which may cause two phase flow conditions at the orifice in the experiment, resulting in a slower pressurization. This deviation from the test specification

will be analyzed in sensitivity analyses (sect. 4.2). The calculated amount of water injected during this phase is 1.58 g, which results from a sudden spike of mass flow rate at 0.79 kg/s.

Phase 2 [200ms - 800ms]: S5 pressurization. The phase starts with the critical flow almost constant at about 0.45 kg/s. No measurement is available for comparison. The calculated pressure in the reaction vessel slightly decreases and then stabilizes at about 11.5-12.0 MPa, which corresponds at the saturation temperature of about 325 °C. The simulation calculates this phase longer than in the experiment. This can be explained with a lower expansion volume in S5 (it is not clearly stated how the level is measured, and its accuracy) and a larger steam flow moving from S1 to S5. A pressure peak of 2.8 MPa is also measured in the expansion vessel at 377 ms, following a sudden steep pressure increase, which seems connected to a sort of CCFL occurrence in the expansion pipe. Indeed, vapor gas, rising in the pipe, expands in S5 because the differential pressure and as consequence of the drag between the fluids may cause the formation of a plug of PbLi acting as temporary piston and, thus, compressing the steam of S5, which cannot condense because the low absolute pressure. This process in the simulation occurs at 600 ms. However, SIMMER-III overestimates the amount of PbLi transported in S5 and the expansion vessel is almost solid, causing pressure oscillations at the beginning of phase 3. The simulation predicts a linear hydrogen generation of about 67.7 g/s, up to 660 ms when the pressures are equalized and the injected water mass flow rate starts to decrease.

Phase 3 [800ms - 6500ms]: S1 and S5 pressures equilibrium. Once S1 and S5 pressures are equalized in the experiment, they increase up to the maximum pressure of 15.0 MPa, occurring when the water injection is stopped. The pressure increase is driven by the water injected, which evaporates, after 3300 ms, in the zone where the chemical reaction affects the melt temperature above the saturation value. The simulation predicts pressure oscillations at beginning of the phase 3 in S5 and a fast pressure increase up to 15.5 MPa, reached at 1000 ms. Once this pressure is reached, the injection stops. From this time on, the hydrogen generation becomes negligible. The code predicts an overall injected water mass equal to 0.367 kg, which result much lower than the value reported in the description document [4].

Phase 4 [6500ms – EoT]: system pressure stabilization. During this phase the injection valve is closed and the parameters are stabilized. The pressures are almost constant (slightly decreasing) in the experiment and in the simulation.

Finally, some considerations about the overall water mass injected and chemical reaction are reported:

- *Water mass injected*. Literature [4] reports that the overall water mass injected in the system is 1.3 kg. This value is unreliable. Considering the volumes of S5 and the injection line, and assuming that all the water evaporates, the calculated water needed to reach

15.5 MPa in saturated conditions is 0.350 kg. Assuming that this water reacts with PbLi producing H₂, the overall pressure is between 10.08 MPa and 20.15 MPa, depending upon the chemical reaction prevailing. It can be concluded that the overall water injected in the system should be larger than 0.262 kg and lower than 0.525 kg. SIMMER-III code estimates a reasonable value being 0.367 kg.

- *Hydrogen generation*. Considering the same assumption, the expected mass of hydrogen generated shall be between 20.4 g and 40.8 g. The results of the simulation is, therefore, acceptable being 31.1 g.



Fig. 3. Run0 "reference" results: pressure in reaction [1,12] and expansion [1,28] vessels compared with experimental data



Fig. 4. Run0 "reference" results: calculated hydrogen generation versus water injection

4.2 Sensitivity calculations and evaluation of the accuracy

Considering the reference calculation (Run0), tens of sensitivity analyses were carried out to understand the reasons of discrepancies between experimental and numerical results. Seven selected sensitivity calculations are reported in Table 2 and fully documented in [10].

Table 2. Sensitivity Test Matrix.

Run#	Modification respect to Run0
Run1	As Run0 without chemical model
Run2	Injection line and expansion tubes
Run3	3" pipe connecting S1 to S5
Run4	As Run3 setting the injection $p = 140$ bar
Run5	U-tube mock-up modeling
Run6	As Run0 with improved heat of reaction
Run7	As Run5, with I&B extrapolated by Test#6

In all the runs, except Run7, it was supposed to inject subcooled water. Nevertheless, after the revision of Test#6 [9], this condition seems to not reflect the real execution of the experiment because of an early rupture of the cap and the consequently two-phase flow injection. Therefore, Run7 was performed imposing a postulated pressure transient from vacuum to 155 bar at the injection device, and the early injector breaks at 53 bar. The sensitivity results are shown in Fig. 5. It can be noted how the pressure transient is more similar to the experimental trend. It might be said that the SIMMER-III code simulation is affected by the correct knowledge of the boundary conditions. In Test #3, these conditions resulting from experimental evidences are not available and can be taken only form test specifications.



Fig. 5. Run7 vs Run0: pressure trends in S1 and S5 and comparison with experimental data.

The evaluation of accuracy plays a relevant role for quantify the reliability and the capability of a code in predicting parameters relevant to safety. This step is a preliminary evaluation based on the application of the FFT-BM developed by University of Pisa ([11]). The results of the FFT-BM, reported in Fig. 6, demonstrate the improvement of the Run7 with respect to the other sensitivities. Indeed, all calculations show values of the reaction vessel average amplitudes rather high (AA > 0.4). The best value is achieved by Run7 (AA = 0.226).



Fig. 6. Average amplitude of S1 pressure accuracy as function of cut frequency by FFTBM

5 Conclusions

The analyses of Test#3 experiment gave the following main results:

- The capability of SIMMER-III code for fusion application in predicting phenomena connected with PbLi/water interaction, considering also the chemical reaction and hydrogen production, has been demonstrated with satisfactory results;

- The consistent post-test analyses permits to improve the knowledge of the experiments, i.e. the water mass injected in the system, the injection pressure trend, and the pressure of the injection cap rupture;

- The sensitivity analyses pointed out the relevance of the initial and boundary conditions on the predictive capabilities of SIMMER-III code to simulate phenomena connected with lithium-lead/water interaction.

Future perspective is to continue the validation process of the modified SIMMER-III code by means of the next LIFUS5/Mod3 experimental campaign in order to obtain reliable and reproducible experimental data with well-known I&B conditions.

Acknowledgments

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

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