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Validation of SIMMER-III code for in-box LOCA of WCLL BB: pre-test analysis of Test D1.1 in LIFUS5/Mod3 facility

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One of the four breeding blanket concepts for European DEMO nuclear fusion reactor is the Water-Cooled Lithium Lead Breeding Blanket (WCLL BB). The WCLL in-box LOCA (Loss Of Coolant Accident) is a major safety concern of this component, therefore transient behavior shall be investigated to support the design, to evaluate the consequences and to adopt mitigating countermeasures. To fulfill this objective, at first, SIMMER-III code was improved by implementing the chemical reaction model between PbLi and water. Then, SIMMER-III Verification and Validation (V&V) procedures have been established and conducted to obtain a qualified code for deterministic safety analysis. The verification activity was successfully completed, while the validation activity requires further effort according to the R&D plan set up in the framework of the EUROfusion Project. In view of this, an experimental campaign and a test matrix has been designed in LIFUS5/Mod3 facility performing pre-test analyses of Test D1.1.

The preliminarily-defined test matrix will be used for the validation SIMMER-III according to a standard procedure. At the present stage, a pre-test analysis was performed to support future experimental tests. In particular, a qualitative analysis of obtained results was performed according to the available data time trends and based on engineering considerations. It aims to interpret the resulting sequence of main events and the identification of phenomenological windows and aspects, relevant to pressure transient and hydrogen production due to the chemical reaction between heavy liquid metal and water.

Keywords: DEMO, WCLL BB, safety, in-box LOCA, SIMMER-III

1. Introduction

The Breeding Blanket (BB) is one of the main components of demonstration (DEMO) reactor. The features of the blanket system can highly affect the safety performance of DEMO reactor [1]. Water-Cooled Lithium-Lead (WCLL) BB is considered among the four alternative options for the European DEMO nuclear fusion reactor [2], [3]. A comprehensive study is conducted in such a way to address the safety response of WCLL BB system in case of a postulated in-box LOCA. Following that, a parallel activity is started, including numerical simulation based on SIMMER-III code and a set of experimental campaigns on LIFUS5/Mod3 test facility, which has been constructed and continually upgraded at ENEA CR Brasimone, Italy [4]. Experimental results will also constitute a useful database for the Verification and Validation of existing codes (refer to [5]) and for the support of new STH/2D coupling calculation tool [6]. The presented work aims to interpret the results of pre-testing phase, which is done according to Test D1.1 and guidelines of the previous numerical and experimental works performed on LIFUS5/Mod2 [7]. A qualitative approach has been used to explain the results and figure out the governing phenomena.

2. LIFUS5/Mod3 description

LIFUS5/Mod3 is a separate effect test facility that consists of rehabilitating and modifying the existed LIFUS5/Mod2 test facility (see refs. [7], [8] for more details) also adding new components such as a new smaller reaction vessel (S1-B). The “test section B” of LIFUS5/Mod3 facility uses the S1-B vessel and will be employed in the framework of EUROfusion program, to investigate the PbLi-water interaction. The main objectives are to investigate the phenomena connected with the physical and chemical interaction between lead-lithium and water, and to validate the chemical model implemented in SIMMER-III code. In connection with these goals, the expected outcomes of the tests are:

- the generation of detailed and reliable experimental data;
- the improvement of the knowledge of thermodynamic and chemical behavior of PbLi eutectic alloy;
- the investigation of the dynamic effects of energy release on the structures, and of the chemical reaction and hydrogen production;
- the enlargement of the database for code verification and validation with a specific focus on the chemical model implemented in SIMMER-III code.

The test section B is designed for higher pressure and temperatures and is employed for studying chemical reaction of lead-lithium eutectic alloy and water. The LIFUS5/Mod3-section B is completely described in [4] and the main components are listed in Tab.1.

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Tab. 1 – LIFUS5/Mod3: vessels design and operating features

Component	Parameter	Value
S1-B Reaction vessel	Volume [m^3]	0.03
	Inner diameter [m]	0.257
	Height [m]	0.5555
	Operating pressure [bar]	>160
	Operating temperature [°C]	480
S2 Water pipe	Volume [m3]	0.004047
	Inner diameter [m]	0.0429
	Design pressure [bar]	200
	Design temperature [°C]	350
S3 Dump vessel	Volume [m3]	2.0
	Inner diameter [m]	1
	Design pressure [bar]	10
	Design temperature [°C]	400
S4-B1 Fresh PbLi	Volume [m^3]	0.40
	Diameter of cylindrical part [m]	0.544
	length [m]	1.56+ ends
	Operating temperature [°C]	400
S4-B2 Depleted PbLi	Volume [m^3]	0.40
	Diameter of cylindrical part [m]	0.544
	length [m]	1.56+ ends
	Operating temperature [°C]	400

3. SIMMER III model

The analytical analyses have been performed with “SIMMER-III Ver. 3F Mod. 0.1”, [9], which is the code version modified at the University of Pisa for fusion applications [10] by implementing the chemical reaction model of the PbLi/Water.

The aim of pre-test simulations is to investigate capability of the chemical model, which is used in SIMMER-III code. Following that, several numerical tests are simulated before starting the experimental campaign [11]. The obtained results from this step will be used in the next steps to support the experimental campaign. For this purpose, two different and precisely defined amounts of injected sub-cooled water in reaction vessel S1-B are considered in the simulations. Five different tests are chosen for pre-test analysis; the test matrix is shown in Tab. 2, including initial and boundary condition of pre-tests.

The reference mesh cell consists of 50 radial and 100 axial cells in the cylindrical coordinates, see Fig. 1 The main SIMMER-III code options of reference calculations are listed hereafter:

- Inter-cell heat transfer applied between all the liquid components and solid particles, in vapor, in the structures, and between structures and liquid components.
- Adjustment of vapor temperature in the two-phase cells with very small void fraction to avoid instability of numerical calculations.
- The properties of the lithium-lead are taken into account from CEA [12], while the properties of the lithium compound were simply set with the available information (Perry’s chemical engineers’ handbook) starting from the properties of the sodium compounds, [13].
- All relevant flags are set in a way that includes turbulence-diffusion term in addition to molecular momentum diffusion (just for the test #4)
- Since SIMMER-III code calculates the friction only in the mesh cells where the “can wall” structures are implemented, in the chemical interaction model calculations the friction in the injection line was neglected.
- The concentrated pressure drops due to geometrical discontinuities are set at the orifice of the injector device.
- Orifice coefficient of enlargement/constriction and curves, implemented in the input file, are calculated by means of empirical correlations as reported in Ref. [14].

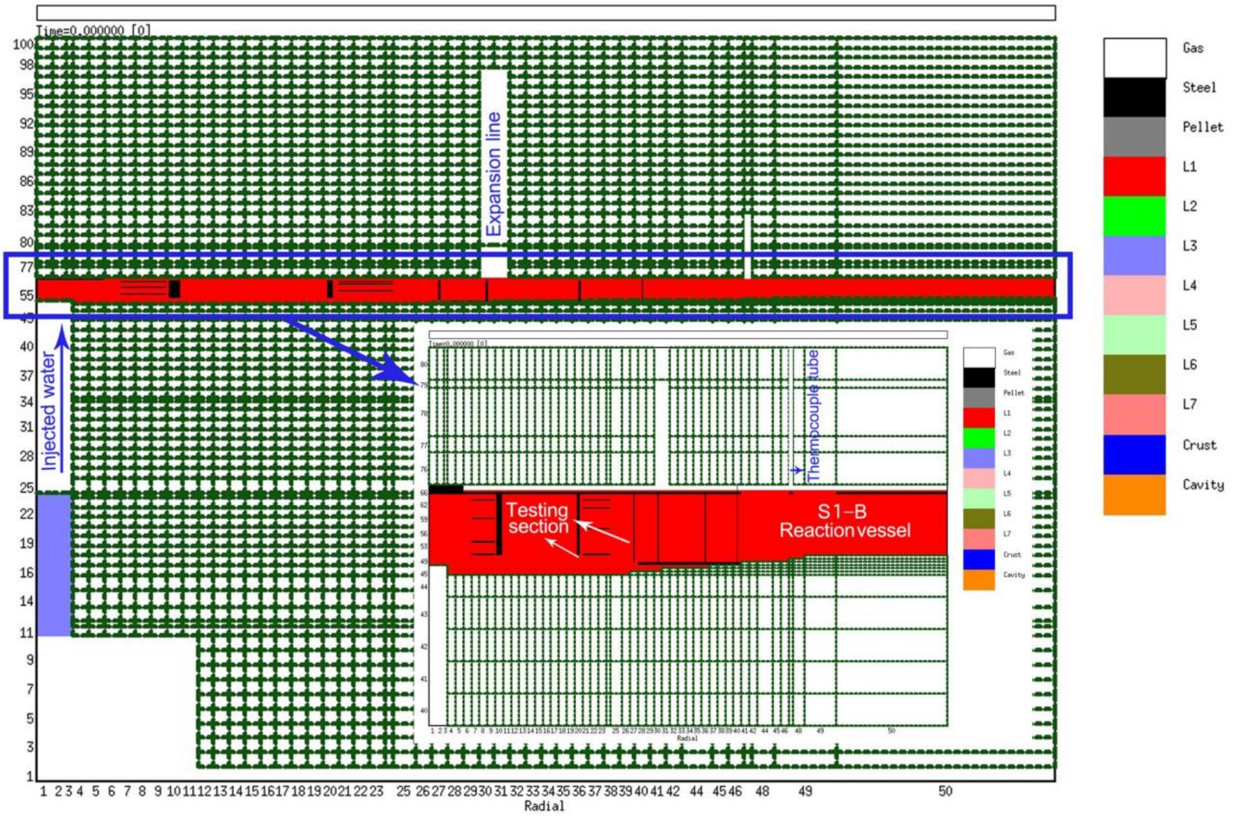

Fig. 1 – Reference mesh cell for SIMMER III mode

Tab. 2 – Pre testing matrix for SIMMER-III reference model; Initial and Boundary conditions

run #	Injected water [g]	T_{H2O} [°C]	$D_{orifice}$ [mm]	T_{PbLi} [°C]	P_{inj} [bar]	P_{vacuum} [bar]	P_{PbLi} [bar]	V_{gas} [m^3]	V_{PbLi} [m^3]	Chemical model	Turbulence-diffusion model
1	**50**	**300**	**4**	**330**	**155**	**0.01**	**1**	**0.00188**	**0.02469**	**Active**	**Off**
2	100	300	4	330	155	0.01	1	0.00188	0.02469	Active	Off
3	100	285	4	330	155	0.01	1	0.00188	0.02469	Active	Off
4	100	300	4	330	155	0.01	1	0.00188	0.02469	Active	On
5	100	300	4	330	155	0.01	1	0.00188	0.02469	Off	Off

4. Results and discussion

The “reference” input deck is labeled “#1”, as reported in Tab. 2. The transient can be divided into four different phenomenological phases. The related time trends and the resulting sequence of events for all pre-tests are reported in (Fig. 2 and Fig. 3).

Phase 1: [from onset of valve opening until the cap injector breaking]: 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. A constant pressure is imposed at the top side of the injection line to simulate the constant inflow of Argon gas from the cylinder through the line, see Fig. 2. The design of the test specifies that the cap should be ruptured at the reference pressure of 155 (bar), therefore the calculation is set by the disappearing of the virtual wall which simulates the injector orifice. In particular, the time rupture is calculated by two-steps: first, the calculation is run with the virtual wall closed to consider the time at which in cell (1,47) the pressure reaches about 155 (bar). Then, the calculation is run again imposing the opening of the virtual wall at that time.

Phase 2: [from 45 to 65 ms]: coolant flashing and first pressure peak.

The water injection and flashing in the liquid metal inside the reaction vessel causes a sudden steep pressure peak. Then the pressure decreases slightly. The injected water presents a spike in pressure shortly after the orifice opening time and then decreases due to the pressurization of the reaction vessel. Nevertheless, water is continuously injected in this phase, indeed the mass flow rate increases again. During phase 2, the hydrogen generated is still negligible, but the value increases during the transient, reaching the equilibrium at the end of phase 3. The results calculated by the code confirm that the chemical reaction in phase 2 is still negligible. In this phase the temperature is more affected by the water cooling effect than the chemical reaction.

Phase 3: [from 65 to 305 ms]: pressurization due to water and gas injection and hydrogen generation, up to pressure equilibrium. This phase can be further divided into two sub-phases, 1) characterized by the water injection and hydrogen production, and 2) characterized by the continuous gas injection up to the pressure equilibrium. To assure that all the water will be injected in the reaction vessel, the design of the tests specifies that a continuous gas flow is injected for all the duration of the experiment in the reaction tank S1-B. This procedure affects the pressure transient in the reaction vessel, which is not anymore driven by the water injection, flashing and chemical reaction, but it permits to exactly evaluate the amount of injected water and therefore to validate the SIMMER-III chemical model.

During the first sub-phase, the pressure in S1-B reaction vessel increases (Fig. 2), driven by the water injected, the water evaporation in the zones where the chemical reaction leads to increase the temperatures above the saturation temperature, and the hydrogen generation. In the meantime, the pressure in the cover gas region increases. Fig. 3 shows the temperature variation at the cell (19,63); the fluctuation is due to chemical interaction of PbLi/water and H_2 production. The maximum temperature is 549°C in test #4.

Phase 4: [from 305 to 2000 ms]: transient ending stage. The phase 4 is characterized by the stabilization of the pressure and temperature in the system (Fig. 2). At this moment, the temperature reaches a stabilized stage close to 330°C and the pressures in the injector and the reaction vessel are equalized, therefore the gas injection is stopped (see Fig. 2 and Fig. 3). On the contrary, due to pressure stabilization, PbLi in the reaction vessel S1-B flow back into the injection line. At the end of the phase 3, the results of total injected water and hydrogen generation are almost fixed.

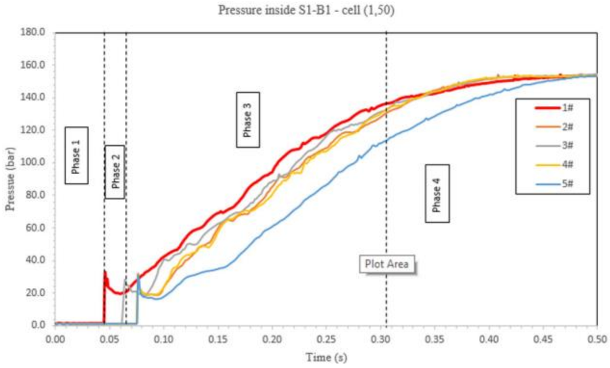

Fig. 2 – Pressure trend; tests number #1 to #5

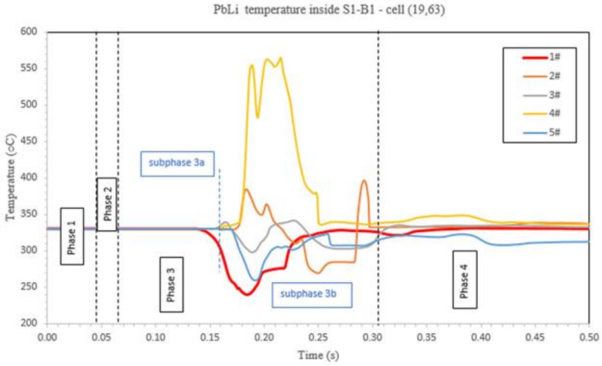

Fig. 3 – Temperature trend; tests number #1 to #5

5. Conclusions

The results of pre-tests can be summarized as follows:

- The most relevant parameters chosen for the definition of test matrix are the temperature of water (from 285°C to 300°C) and the mass of injected water (from 50 g to 100 g).
- Mass of injected water directly influences the hydrogen production and the melt temperature.
- The maximum temperature and hydrogen production are reached with 100 g of injected water.
- The pressure of cover gas shows a peak and a low oscillating behavior due to the piston effect of the injected gas. The effect of gas compression in the system is more noticeable considering the pressure in the hydrogen extraction line.

Final pressure in S1-B reaction vessel is not correlated to the considered parameters but is affected by the need of injecting all water in the reaction vessel, thus keeping the argon gas and the injection valve opened up to the pressure equalization (i.e. imposed in the calculation).

Acknowledgments

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