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SIMMER-III/ANSYS coupling
(Preliminary development and validation activities of an integral tool for the design and analysis of WCLL components)

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Abstract
In the framework of the development of fusion energy, one of the most prominent technologies arising to address the issues of tritium breeding and power conversion is the Water-Cooled Lithium-Lead (WCLL). This technology utilizes a molten eutectic alloy of Lithium and Lead which circulates inside the Breeding Blanket (BB) and is irradiated with neutrons to produce tritium. Water is then circulated inside the system to cool the components. The simultaneous presence inside critical areas of the reactor of molten metal alloy and water, at high temperature and pressure, poses significant safety concerns. For this reason, adequate design and analysis techniques are required to ensure the ability of the system to survive and mitigate any possible damage in case of the in-box Loss of Coolant Accident (LOCA), the most critical postulated accidental scenario. With this aim in mind, a novel approach was implemented with the aim of coupling the SIMMER-III code and the ANSYS Mechanical code for the modelling of both the chemical and thermodynamical interactions between water and the alloy, and the resulting effects on the structures. This work presents the status of the coupling technique development and the results of the preliminary validation activities performed against experimental data provided by the LIFUS5 facility operating at ENEA Brasimone Research Centre. The resulting comparison between these data and the codes' predictions allows a careful evaluation of the errors introduced in each step of the chain. Moreover, it provides confidence in the capacity of the methodology to correctly predict the ability of the structures to withstand incidental loads without suffering extensive damage.

This work aims at providing engineers with a usable and powerful tool that allows for the safety analysis of WCLL-based components during the early stages of the design phase. This would help save time, and effort and reduce the economic cost that might arise from any undetected issue propagating downstream the design process.

Keywords : Water-Cooled Lithium-Lead (WCLL), In-box Loss Of Coolant Accident (LOCA), ITER, DEMO, Breeding blanket, Numerical simulation

1. Introduction

In the framework of fusion energy development, one of the main designs proposed for the implementation of the breeding blanket module is the WCLL (Water-Cooled Lithium-Lead). This technology aims at solving the tritium supply and power conversion issues in fusion reactors by circulating in the breeding blanket a molten eutectic alloy of Lead and Lithium (PbLi), which is in turn cooled by flowing water (Boccaccini et al., 2022; Cismondi et al., 2020; Martelli et al., 2018; Tassone et al., 2018). However, the simultaneous presence in the system of high-pressure water and high-temperature reactive alloy poses significant issues that must be extensively investigated to ensure operational reliability and comply with safety standards. One of the most critical scenarios in this respect is the in-box LOCA (Loss Of Coolant Accident), in which one of the water cooling pipes is supposed to rupture inside the breeding unit.

In the past, extensive effort was put into investigating the response of the WCLL-related systems to such scenarios, both from the experimental point of view (Eboli et al., 2019, 2021; Moghanaki et al., 2020) and by developing dedicated numerical tools and analysis methods(Galleni et al., 2021; Moghanaki et al., 2019, 2021). These activities aim to provide designers with a wide range of tools that allow them to perform a complete integral safety analysis of the whole system and ensure its compliance with the strictest safety standards.

Up to this date, the numerical code development activities focused on the implementation of the chemical models that simulate the interaction between water and PbLi inside the SIMMER-III code (Galleni et al., 2022; Pesetti et al., 2016) and on the development of code chains to study the hydraulic behaviour of the system in these scenarios (Galleni et al., 2020; Pesetti et al., 2016; Pucciarelli et al., 2021). However, all these codes and code chains focused on the goal of simulating the behaviour of the fluid part of the system, neglecting the response of the structures under these dynamical loadings.

This work introduces a new activity, which aims at solving these issues by coupling the SIMMER-III code, which is a 2D, multiphase and multicomponent, Eulerian, fluid dynamics code, and the ANSYS Mechanical code, used for the simulation of the mechanical behaviour of structures and systems. Moreover, this work presents the preliminary V&V activities performed on the structural side of the code chain. The final scope of this activity is to provide designers with the last tool needed for the complete analysis of the thermohydraulic and mechanical behaviour of the systems during incidental scenarios.

In the following sections a detailed description of the status of the code development, and the verification and validation activities performed up to this point will be presented. The simulation outcomes will be discussed and compared with experimental data from the database generated by experimental campaigns performed at the ENEA Brasimone Research Centre on the LIFUS5/Mod2 and Mod3 facilities (Badodi et al., 2022).

2. Nomenclature

BB	Breeding Blanket	V&V	Verification and Validation
LOCA	Loss of Coolant Accident	EoI	End of Injection
TBM	Test Blanket Module	PC	Absolute pressure transducer
WCLL	Water-Cooled Lithium-Lead	PT	Fast pressure transducer
RC	Research Centre	PbLi	Lithium-Lead alloy

3. Materials and methods

The code chain described in this work will be based on two numerical codes, the SIMMER-III code (SIMMER-III Ver.3F modified by ENEA and UNIPI), and the ANSYS Mechanical code (ANSYS® Mechanical 2022 R1, n.d.).

The first one will be used to simulate the interaction between water and PbLi, and it will provide information on the thermodynamic parameters involved during the incidental transients. This code was chosen due to its ability to simulate both the thermodynamical interaction between the two fluids, as well as the chemical interaction occurring at the specific temperatures and pressures, thanks to the extensive implementation work performed in the past (Eboli et al., 2016). Moreover, the code was validated extensively thanks to the datasets created during experimental activities at ENEA Brasimone RC on the LIFUS5/Mod3 facility (Badodi et al., 2022; Eboli et al., 2020; Moghanaki et al., 2019, 2021).

The structure response to the pressure transients generated during the interaction will be simulated by the ANSYS Mechanical code. This software was chosen for its stability, simplicity of use, and variety of models implemented. The Mechanical application allows the user to perform both static and dynamic analysis of structures with high precision and with a small effort compared to non-commercial codes.

The described activity aims at obtaining a fully automated coupling between the two codes, with the coupling tool automatically taking care of streamlining the data between them.

3.1 Code chain validation: methodology and data

The verification and validation activities will follow the schematic shown in Fig. 1. Firstly, the SIMMER-III code, which implements the chemical and thermodynamical models of the PbLi-water interaction, has been extensively validated against experimental data (Galleni et al., 2022).

This validation activity allowed the complete evaluation of the error committed when simulating a real system with this code. The scheme refers to this error as Δ_1 and all these validation activities are extensively described in the literature.

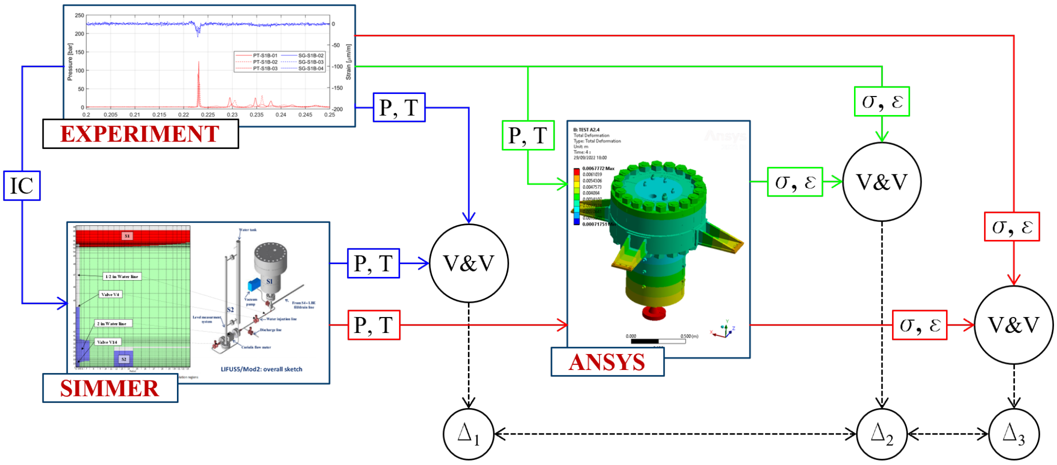


Fig. 1 General outline of the verification and validation activities foreseen for the code chain methodology. The experimental data are used to validate singularly the output of the SIMMER-III code (blue path) and of the ANSYS Mechanical models (green path). Then, the full code chain is validated against them (red path). The errors calculated this way can be used to identify the steps of the chain that need better calibration and enhancement.

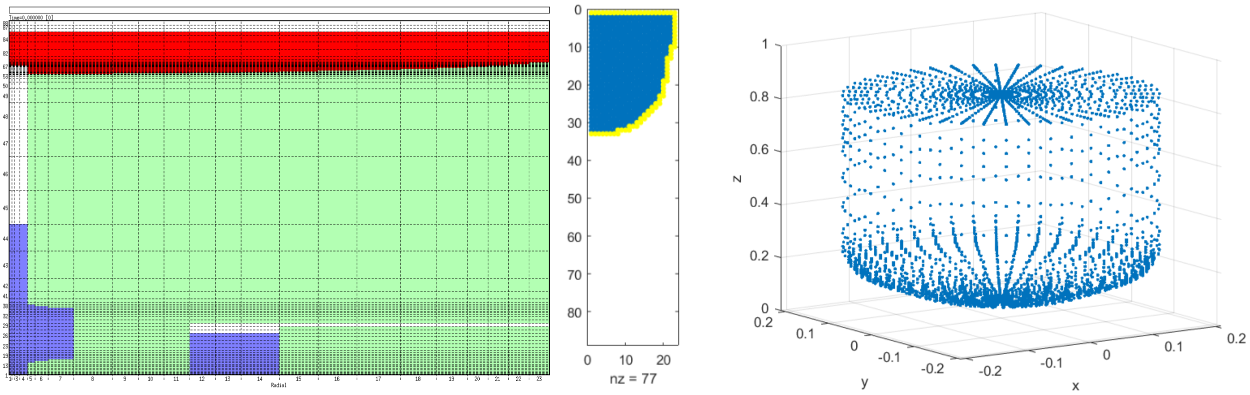
After this first step was completed, the focus shifted to the verification and validation of the simulations performed with the ANSYS Mechanical code. To do so, several simulations are foreseen to be carried out, replicating the same conditions of tests performed on the facilities that have been operated at Brasimone Research Centre and for which an extensive database collecting all the needed data is available. This database includes test performed on two different configurations of the LIFUS5/Mod2: THINS and LEADER. They provided extensive data on the thermodynamical interaction of water and Lead-Bismuth eutectic alloy (Del Nevo et al., 2019; Pesetti et al., 2016) with pressures ranging between 40 and 180 bars and temperatures of 400°C. Although this alloy is not utilized in fusion reactors, validation will be carried out also on these data for two main reasons: the results can be compared with previous modelling work (Di Maio et al., 2019) to gain confidence in their quality, and the validation can be performed on a wider database including different geometries. A second set of data comes from the LIFUS5/Mod3 facility (L5M3) which was instead operated using PbLi simulating LOCA events with pressures of around 180 bar and temperatures ranging between 300 and 400°C (Badodi et al., 2022; Eboli et al., 2019). The data provided will be utilized in further steps of the validation activities.

Each configuration of the facility is equipped with a set of sensors that allow the correlation of the experimental results with the numerical ones. Inside the vessel, pressure transducers continuously monitor pressure and pressure wave generated by the fluid interaction, while strain gauges mounted on the vessel wall allow the characterization of its deformation during the tests.

For validating the code against a test, the exact geometry of the system is modelled using CAD software and simulated with the ANSYS Mechanical code. The readout of the pressure sensors inside the vessel is used as a boundary condition during the simulation, while the readouts of the strain gauges are then compared to their numerical equivalent. This comparison between the experimental data and the ANSYS Mechanical code alone allows the evaluation of the error introduced during the mechanical simulations, which in Fig. 1 is referred to as Δ_2.

The last step of the validation process lies in the evaluation of the precision of the whole chain. With this respect, one or more of the tests will be simulated without the usage of the experimental data but using only the codes in future activities. With this respect, the SIMMER-III code will evaluate the pressure transient inside the vessel starting from the geometry and initial condition of the system. Then the ANSYS Mechanical code will evaluate the deformation caused on the vessel. This output is then compared with the experimental output, leading to the error evaluation in Fig. 1 referred to as Δ_3.

By performing this extensive validation activity, the individual error committed by each code is known (Δ_1 and Δ_2) and the total error committed by the chain, allowing the identification of criticalities or steps viable for optimization.



(a) (b) ©

Fig. 2 Working principle of the coupling tool: a) the data generated by the SIMMER-III code is imported in the tool. Green: non-calculation zone, White: Argon zone, Blue: water zone, Red: PbLi zone; b) The boundary of the PbLi region is detected and added to a selection mask. Blue: PbLi zone, Yellow: boundary selection mask; c) The boundary cells are expanded in the 3D space by replicating them at each angular step. This converts the grid of SIMMER-III to a point cloud suitable for the import into ANSYS Mechanical.

3.2 Coupling tool development

The coupling tool is currently under development using a combination of MATLAB and the integrated IronPython engine included with the ANSYS distribution. A MATLAB script is used to extract the information included in the SIMMER SIMBF output and to post-process the data, as shown in Fig. 2a. The mesh and data import is obtained via a function that reads the SIMMER-III binary output, developed by UNIPI. Once the data are loaded in MATLAB, an edge-detecting convolution algorithm is applied to the node matrix to individuate the fluid region and extract the surface of the calculation zone.

The result is shown in Fig. 2b where the yellow dots represent the mesh nodes detected as borders. This algorithm is based on a simple convolution with a uniform 3x3 kernel and subsequent matrix thresholding, to generate a selection mask. Once the mesh boundary is detected, the mesh is expanded in the 3D space by replication along the toroidal direction (Fig. 2c), and the pressure values on the boundary are mapped onto the new mesh. The outcome of this algorithm is a point cloud in which each point contains the x, y, and z coordinates and a pressure value for each timestep. The data are exported in CSV files that can then be imported into ANSYS Mechancial using the "External Data" interface and applied to the simulation setup. The point cloud is mapped by the simulation engine onto the mesh and the pressure is applied as a boundary condition. Currently this last step is manual, but it will be automatized by designing a suitable piece of software using the IronPython engine during the next steps of the development activities.

3.3 Status of the validation activities

At the current time, validation activities are advancing through a first phase in which the performance of the ANSYS Mechanical code is being evaluated against time-varying experimental data, while a first steady state validation has already been completed. The next paragraphs will describe in detail the configuration of the LIFUS5/Mod2 THINS facility used in this first validation phase and the simulation setup on which the activities focused. The data utilized refer to the tests A-1.4, A-2.3 and A-2.4, where the first two test were simulated only in the steady state regime, comparing the results with the state of the facility at the end of the test, while for the third one both steady state and transient simulation were performed.

Three steady-state analyses have been performed to validate the geometrical, boundary conditions, and load application sequences implemented for the simulation. These simulations consider only the vessel constraints and the initial and final pressures and neglect both time integration and the variation of the load during the transient phase of the test. Dynamical simulations instead consider all the constraints and pre-loading phases but also implement a time integration scheme and the full-time varying pressure profile inside the vessel for the test sequence of interest.

3.4 LIFUS5/Mod3 in the THINS configuration: layout and test description

The LIFUS5/Mod2 facility in THINS configuration is primarily composed of the main reaction vessel shown in Fig. 3. This vessel is made of Tp. 316 stainless steel and is designed to withstand a pressure of 200 bar at 500°C. Its internal volume is 100 L.

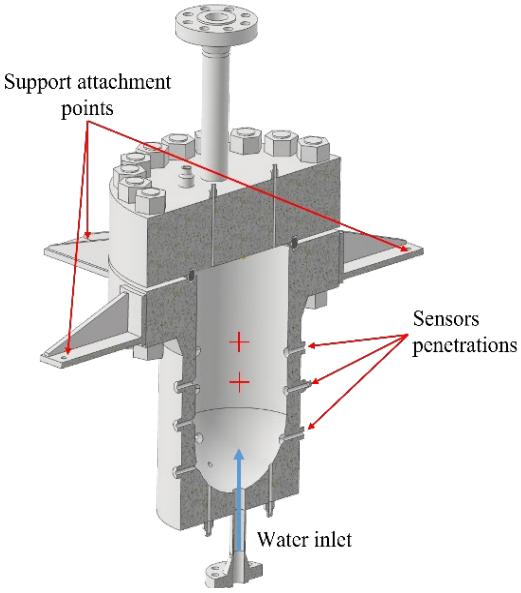


Fig. 3 LIFUS5/Mod2-THINS configuration reaction vessel, cut isometric view. Red crosses: strain gages placement on the inner wall.

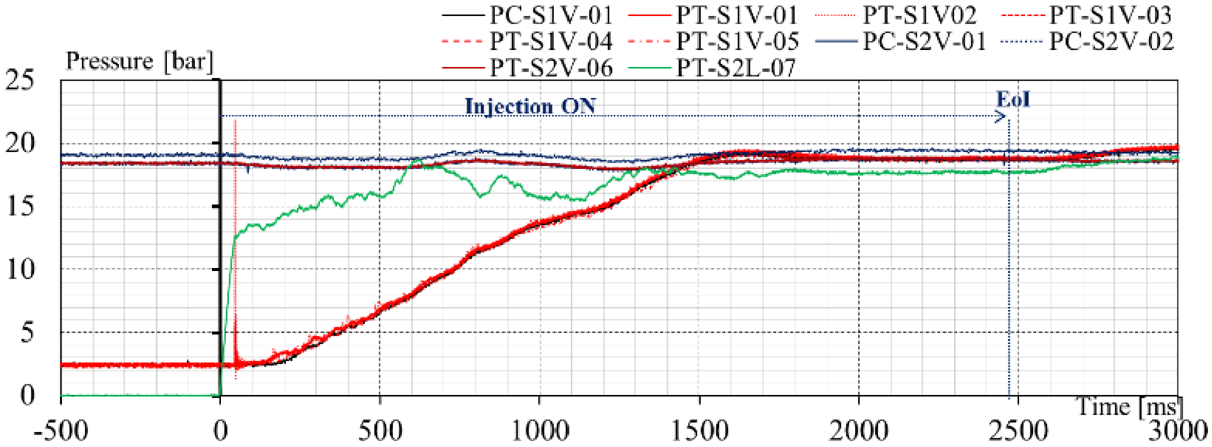


Fig. 4 Sample data acquired from the pressure and strain sensors in the reaction vessel and injection line.

During a test, the vessel is filled with molten alloy up to a predetermined level, while the rest is filled with inert gas. The whole system is isolated and heated via electric cables to maintain a fixed and pre-determined temperature. Water is then injected into the alloy via an injector device that is inserted in the vessel passing through the bottom flange allowing the simulation of water leakage or pipe rupture events. Several sensors are placed inside and outside the vessel to monitor all the relevant parameters, including thermocouples acquired at 50Hz, pressure transducers and strain gages acquired at 1kHz. An example of the acquired data is shown in Fig. 4, where the traces represent the acquired pressure signal from different transducers placed in the vessel and injection line. The injection phase is highlighted to show the pressure trends during the test.

The most important sensors used during the validation activity are the pressure transducers and the strain gauges. The first sensor is used to monitor the pressure variation inside the vessel while the second measures the deformation of the vessel walls under these conditions allowing the correlation between the two measurements. Both sensors acquire data at 1 kHz to resolve the fast pressure transients that occur immediately after the water injection due to flashing and vaporization.

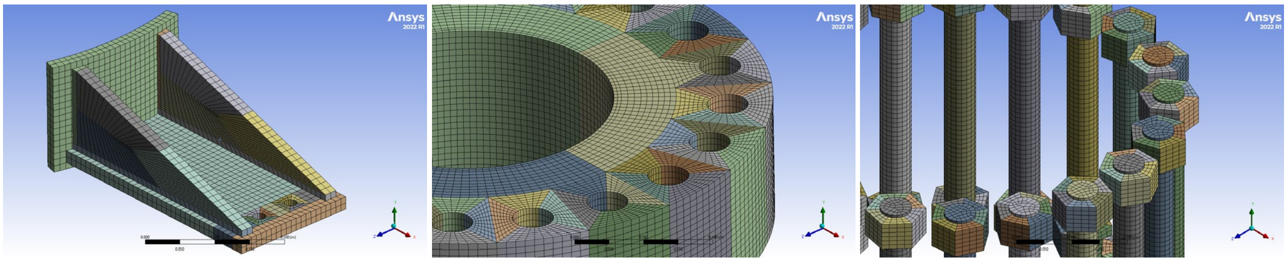
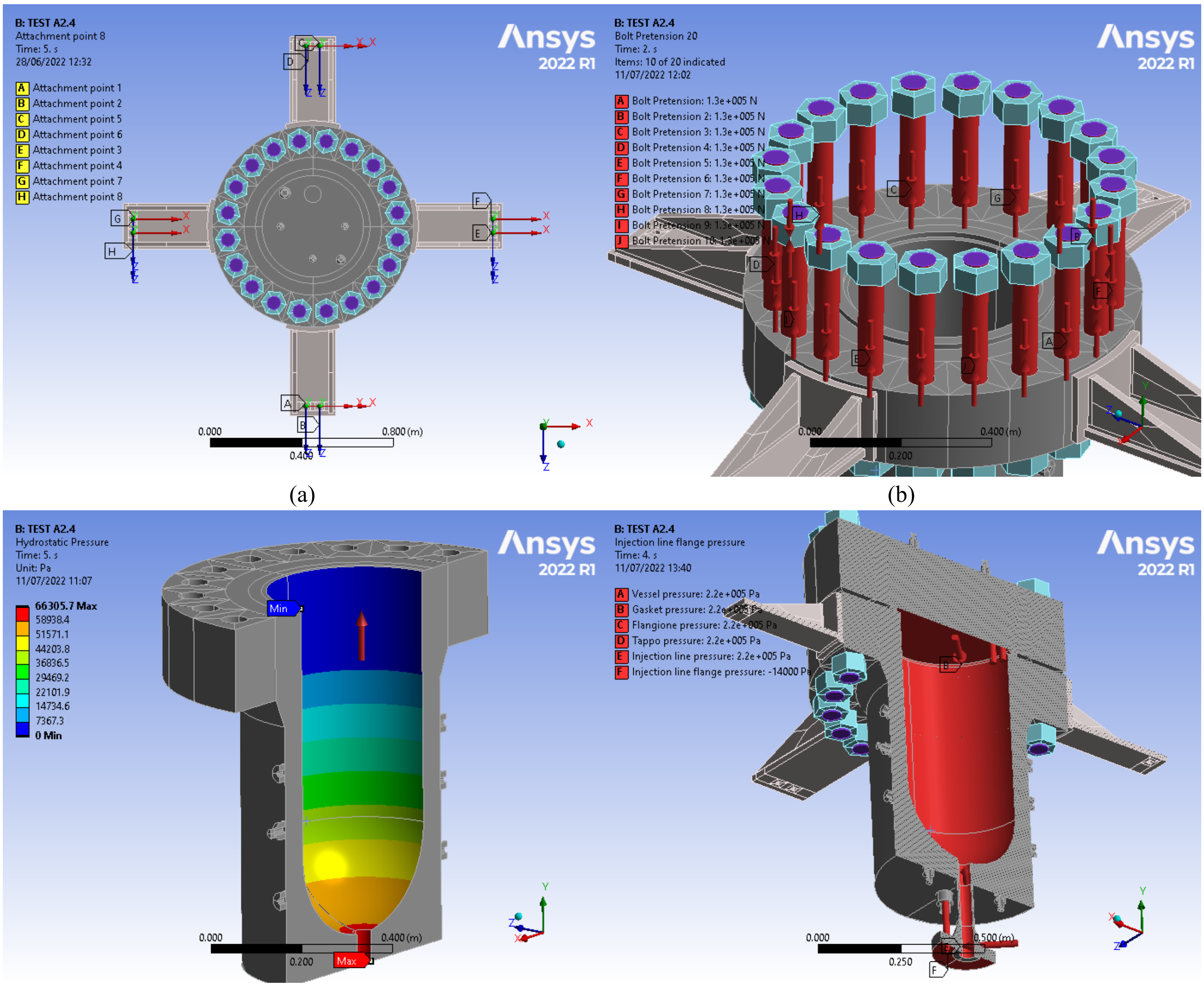


Fig. 5 Mesh generated for various vessel zones. a) Support saddles; b) Top flange and bolt holes; c) bolts and nuts.



(a) (b)

(c) (d)

Fig. 6 Loads applied to the ANSYS Mechanical model for simulating the static response of the structure. a) Constraints on the attachment points can move outward but can't move out of plane nor rotate around the in-plane axes. b) Preload is applied to the bolts to simulate flange assembly and tightening. c) hydrostatic pressure due to the presence of the PbLi is applied to the inner surface of the vessel. d) Inner pressure is applied to simulate the steady state condition of the vessel after a test.

To validate the model and simulation setup, a replica of the geometrical model of the facility was built and meshed in the ANSYS Mechanical application. The mesh was built to be as regular and high quality as possible to exclude numerical errors introduced in this phase and it is shown in Fig. 5. The geometry was simplified to avoid the overcomplication of the model and the simulation of components that do not significantly impact the outcome. For this reason, the lateral penetrations in the vessel have been removed, and the holes for the passage of the sensors filled. Also, the top line has been removed, since, in the THINS configuration, it was plugged with a metal disk. These operations allowed the regularization of the domain and thus the generation of a higher-quality mesh.

Another point that was considered during this validation activity was material properties. All the materials that comprise the facility are known, and their properties were considered complete of their temperature dependence over the whole range of temperatures.

Fig. 6 shows a recap of the constraints and loadings applied to the vessel. The supports are constrained to avoid lateral sliding of the system, as well as its rotation, but can slide radially to allow thermal expansion during the heating phase. Gravitational acceleration is considered for the system to simulate the weight of the vessel and the flange, that in this case is not negligible. Hydrostatic pressure applied on the internal surfaces simulates the presence of the PbBi alloy.

Contacts in the system are all set as “bonded”. This is done to simplify and speed up solution calculation but introduces some discrepancies between the real and numerical system, since friction exists between any metal-metal contact, with a coefficient of around 0.3. However, the only contact points between the bodies are:

- Contact between the vessel, the top flange, and the gasket separating the two;
- Contacts between the nuts, the flange, and the vessel;
- Contact between the nuts and the bolts.

Modelling the gasket using a bonded contact instead of frictional will not introduce much distortion in the solution, since the gasket is locked into a groove and cannot move. Nuts and bolts are locked onto each other via the threads and once tightened they are expected not to move, thus they can be approximated as bonded. The last remaining contact is the one between the nuts, the vessel, and the top flange. It might be expected that during the tightening procedure some displacement could occur in these points, however, due to the dimension and stiffness of the involved components no significative distortion of the solution is expected in this regard.

Before any pressure loading is applied to the system pre-tensioning is applied to the bolts, to prestress the flange to the vessel. Any subsequent timestep considers the bolts locked. At last, on the internal surfaces, the pressure due to the PbBi-Water interaction is applied and the structure is simulated.

The loading sequence utilized in the simulation mimics the actual loading sequence implemented in reality: gravity loads are applied at step 1, together with the support constraints. Then in step 2 bolts are tightened and locked. After this, in step 3, the temperature rises, and during step 4 the initial internal pressure at the beginning of the test is applied. The next step depends on whether the analysis is static or dynamic. In the first case, just one more step is configured, with no time integration, to apply the internal pressure at the end of the transient phase, when the system has reached equilibrium. In the other case, the whole sequence of the pressure transient is applied, and time integration schemes are included in the model. In this case step 5 is utilized as a buffer step where time integration schemes are turned on, but the pressure is constant. This allows the stabilization of the solution, which tends to oscillate right after the time integration steps are introduced.

After the end of the simulation, the strain field is calculated and sampled at the same points and in the same direction as the installed strain gauges. All the strain gauges mounted on the vessel are oriented according to the hoop direction, to accurately measure the hoop strain of the vessel wall.

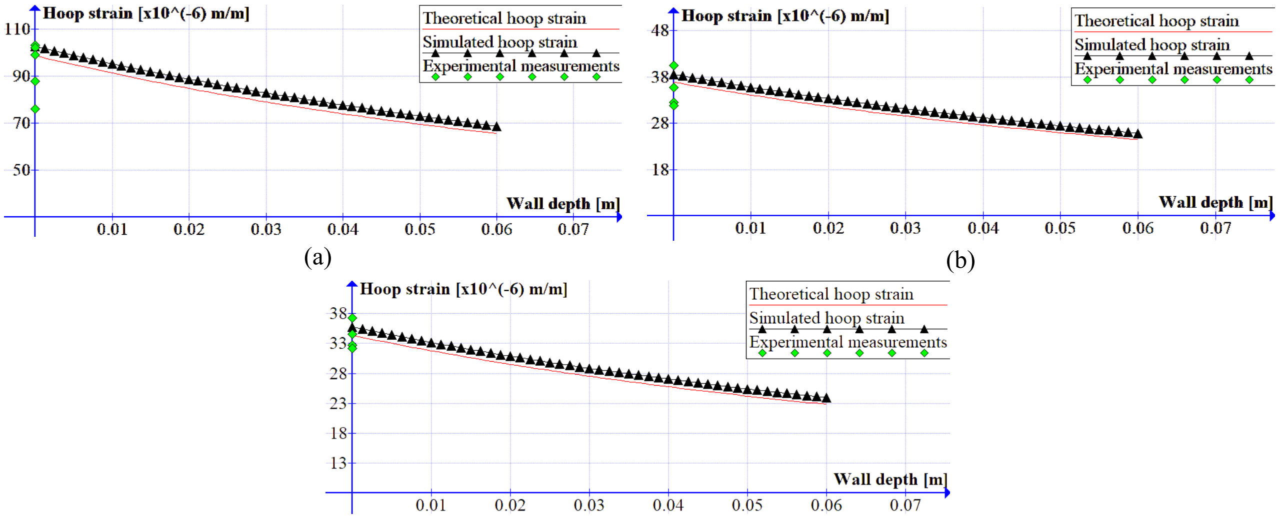
The numerical solution is compared with both the experimental and the theoretical results. In particular, the hoop strain field inside the vessel wall can be calculated according to the formula:

$$\varepsilon_\phi = \frac{1}{E}\left[(1+\nu)(p_i - p_e)\frac{R_e^2 R_i^2}{R_e^2 - R_i^2}\frac{1}{r^2} + \frac{1-2\nu}{R_e^2 - R_i^2}\left(p_i R_i^2 - p_e R_e^2\right)\right] + \alpha\theta \tag{1}$$

where: E is the material elastic modulus; ν is the material Poisson’s ratio; p_i and p_e are respectively the internal and external pressures; R_e and R_i are the external and internal radiuses of the vessel wall; r is the radial coordinate along the vessel wall; α is the linear coefficient of thermal expansion; θ is the temperature variation between the initial and final state of the system, which in this case coincides just with the temperature difference between ambient temperature and the uniform test temperature.

4. Results and discussion

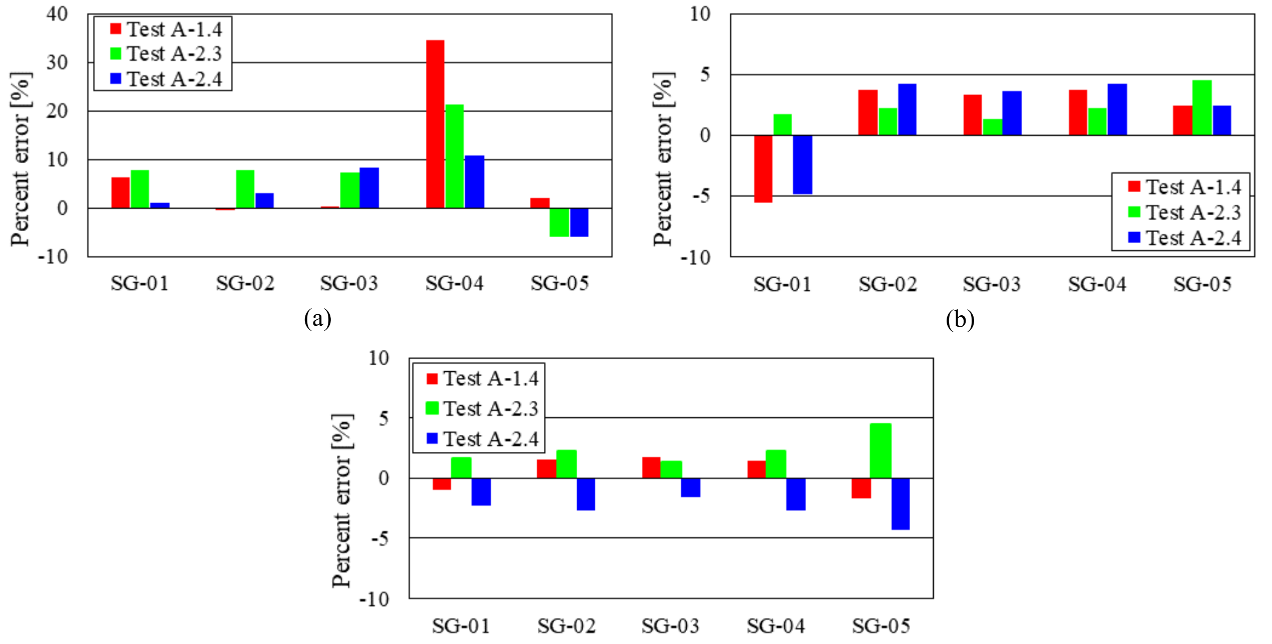
In this section results from the static and dynamic validation against tests performed on the LIFUS5/Mod2 in THINS configuration are reported. Moreover, in Paragraph 4.3 a brief description of the results of the mapping algorithm between the SIMMER-III and ANSYS Mechanical meshes is reported.



(a) (b)

(c)

Fig. 7 Results from the static validation activity: comparison of the stress profile inside the vessel wall between numerical (black triangles), experimental (green squares) and theoretical (red line). a) test A-1.4; b) test A-2.3; c) test A-2.4.



(a) (b)

(c)

Fig. 8 Analysis of the steady-state percent error between the ANSYS Mechanical simulation and: a) experimental results; b) theoretical results and c) previous numerical simulations (Di Maio et al., 2019)

4.1 Static results

Fig. 7 shows the comparison between experimental, numerical, and theoretical values of the hoop strain across the wall of the vessel for the tests A-1.4, A-2.3 and A-2.4 obtained from the static simulation. The data shown along the ordinates axis represents the hoop strain compared to the deformation at the beginning of the test (numerical step 4). This means that the values are calculated according to the formula:

$$\text{Hoop strain} = \epsilon_{\Phi}(EoT) - \epsilon_{\Phi}(SoT) \tag{2}$$

where EoT and SoT represent:

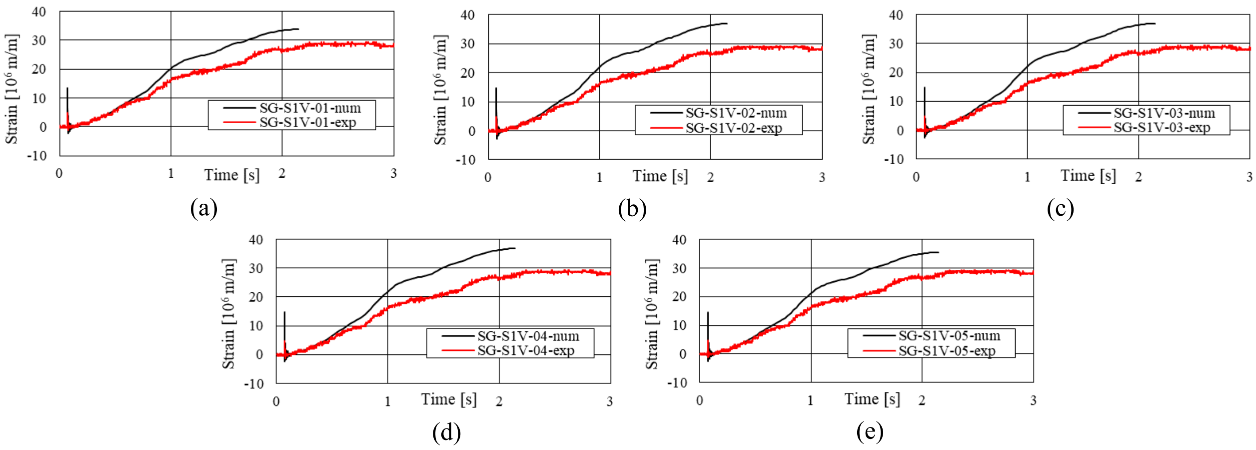
- The beginning of the injection and the end of the acquisition time for the experimental data;
- The first timestep in which pressure is applied and the last timestep of the simulation for the numerical results.

By subtracting data relative to the first instant of the test, eventual offset on the sensors or the simulation results are compensated, and the results can be easily compared.

The numerical and theoretical hoop strain along the vessel wall depth show only a small offset, while experimental data are more scattered around due to the uncertainty associated with their acquisition.

For a better visualization of the error committed by the simulations, Fig. 8 shows a comparison between the hoop strain at the strain gauges positions (see Fig. 3) extracted by the gauges data, the theory, the numerical simulations, and the results obtained in the previous work (Di Maio et al., 2019). We can see how, for most of the sensors, the numerical-experimental error lies lower than 10% with only SG-04 showing a higher value during tests A-1.4 and 2.3. Percent error between numerical and theoretical data instead lies around ±5% for all the tests, giving confidence in the quality of the numerically generated data, and the error between the simulations obtained in this work and in previous ones lies always under ±5% showing consistency and accuracy of the numerical methods in simulating such scenarios.

4.2 Dynamic results



(a) (b) (c)

(d) (e)

Fig. 9 Transient time simulation results comparison between the readouts of the real and virtual strain gages placed at matching positions in the vessel. a) Strain gage 01; b) Strain gage 02; c) Strain gage 03; d) Strain gage 04; e) Strain gage 05.

The previous static validation activity confirmed the quality of the numerically generated data and provided confidence in the method with which the system's model in ANSYS Mechanical was set up. The next step consisted of performing a transient-time simulation using the full set of data provided by the facility. With this regard, the same simulation setup was transposed to a transient-time simulation that used the pressure trend of test A-2.4 as input.

The results of this analysis are shown in Fig. 9. Each graph shows the transient time response of one of the strain gauges mounted inside the vessel together with its numerical counterpart. It can be noted how the numerical simulation can closely follow the strain trend measured by sensors, with a precision that is very high at the beginning of the transient and then diminishes towards the end. This discrepancy can be easily explained by the fact that during the interaction temperature inside the vessel rises and the vessel walls are slowly heated, causing an outward dilation. This effect is not taken into account in the simulations yet, but it will be implemented in the future.

A zoom on the first peak area for SG-02 data is shown in Fig. 10. From the graphs, it can be noted how the experimental readout of the peak is distorted if compared to the numerical evaluation. This is due to the low sampling frequency of the signal, which is acquired at only 1 kHz. However, from the graph, it can be noted how even the fast transient right after the injection is resolved adequately by the numerical simulation, and the main frequencies and the damping time are well captured.

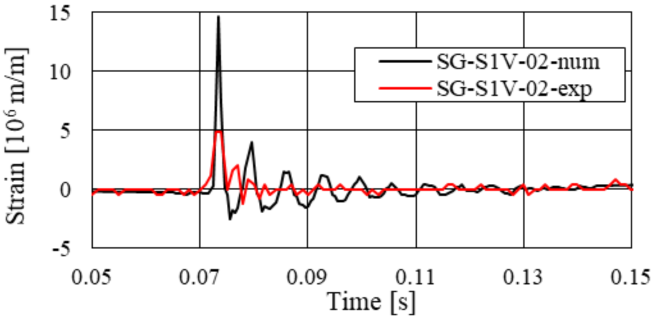


Fig. 10 Transient time simulation results, zoom on the 50-150ms interval. The figure shows how the sampling rate of the sensors is clearly not enough to follow the fast transient dynamics.

5. Conclusions

This work aims at introducing the novel code coupling activity developed to simplify and enhance the work of designers, providing them with a tool for the integral optimization of WCLL-related components, and presenting the preliminary validation activities which are being carried out on the tool.

To ensure the quality of the results, a wide validation activity is being carried out utilizing the data generated during years of experimental activity at the ENEA Brasimone Research Centre. Steady-state simulations of the LIFUS5/Mod2 THINS facility show good agreement between experimental and simulated output. The same comparison was performed utilizing time-transient data, again showing good agreement between numerical and experimental readouts, even if some issues with the sampling frequency of the signals are detected in the data.

Several critical points have been discussed in this work, and it was pointed out how the current validation was performed mostly using data from facilities that are not operated using PbLi. To address these issues, the work will be expanded to include solutions to all of them: firstly, by simulating a different dataset with fast-acquired (10 kHz) experimental data. Then, by simulating experimental campaigns performed on the LIFUS5/Mod3 facility, which uses PbLi as the working fluid. The thermal behaviour of the system will also be included in future models to keep into consideration the thermal expansion effects on the structure integrity.

Moreover, during the next few months, the coupling algorithm will be expanded and enhanced. to remove the need for extensive user setup and to add support for 3D meshes and, at last, the whole code chain will be implemented and validated, to address any step introducing error in the pipeline.

Overall, the results presented in this work provide confidence about the quality that can be obtained with this method and the capacity of the code chain to enhance designer's ability to simulate and optimize WCLL components to meet the most stringent requirements for their operation.

Acknowledgements

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