Fusion Engineering and Design 153 (2020) 111504

Contents lists available at ScienceDirect

Fusion Engineering and Design

journal homepage: www.elsevier.com/locate/fusengdes

RELAP5/SIMMER-III code coupling development for PbLi-water interaction

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ARTICLE INFO

Keywords:
Coupling codes
SIMMER-III code
RELAP5 code
WCLL
PbLi

ABSTRACT

A major safety issue in the Water-Cooled Lead-Lithium Breeding Blanket (WCLL-BB) system foreseen for fusion reactor is the interaction concerning the primary coolant (water) and the neutron multiplier (PbLi), due to a hypothetical tube rupture in the coolant circuit. This scenario involves an exothermic chemical reaction between PbLi and water with the production of hydrogen, in addition to critical interactions in a complex multiphase system in non-thermal equilibrium. In recent years the PbLi/water reaction was successfully implemented in the SIMMER-III code and validated against data from the LIFUS5/Mod3 experimental campaign. However, due to limitations of SIMMER-III, this work was restricted to the prediction of the phenomena inside the vessel, neglecting the simulation of the injection line. Nevertheless, since the injection line may actually have an important effect on the development of the transient, the simulation of the whole facility would be highly desirable. Indeed, the University of Pisa recently developed a coupling methodology between the SIMMER-III and RELAP5/Mod3.3 codes and applied it to simple single-phase cases. In this paper the complete simulation of the LIFUS5/Mod3 facility is presented, with the injection line modelled through RELAP5. Furthermore, all the complex aspects of the phenomena inside the reaction tank were included: the multiphase system and the interaction between water and PbLi with the chemical reaction and the production of hydrogen were modelled by SIMMER. Preliminary results are presented, showing that the coupling methodology can be effectively employed for the prediction of the chemical and thermal-hydraulic behaviour of complex loop experimental facilities.

1. Introduction

Thermal-hydraulic and safety analyses are a central issue in the advance, design and licensing of nuclear power plants (NPPs). Particularly, the study of the plant behaviour in accidental situations has always been one of the chief concern of nuclear safety. These investigations are essential to assess the consequences of a postulated accident and to assist the design of the facilities in order to assure the structural integrity of the components, or, furthermore, to avoid putting at risk the whole system.

One of the major safety issues regarding the Water-Cooled Lead-Lithium Breeding Blanket (WCLL-BB) for the fusion DEMO (DEMOnstration Power Station) reactor is the interaction between the primary coolant (water) and the neutron multiplier, i.e. Lead-Lithium alloy (PbLi), due to a rupture in the coolant circuit [1–3]. This accident scenario involves an exothermic chemical reaction between PbLi and water with the production of hydrogen, in addition to critical interactions in a complex multiphase system in non-thermal equilibrium, which may lead to a vapour explosion and pressurization of the vessel.

To simulate this scenario the SIMMER-III code was chosen, since it is able to simulate multiphase systems involving phase transitions and several materials, including liquid metals. Furthermore, SIMMER-III can be modified to simulate chemical reactions between water and different liquid metals: the University of Pisa successfully implemented a PbLi/water reaction model in SIMMER-III, permitting the estimation of the energy release and the hydrogen generation [4]. Validation activity on the obtained data is ongoing on experimental tests in the LIFUS5/Mod3 (LIthium for FUSion) facility at the ENEA (Italian National Agency for New Technologies, Energy and Sustainable Economic Development) Brasimone Research Centre (Italy) for the EUROfusion project [5–7].

However, simulation of the whole facility solely with the SIMMER-III code remains impractical: firstly because SIMMER-III operates better with axial-symmetric domains (since it was originally developed for core accident analysis) and therefore it is not fully suitable for the simulation of complex pipeline systems, such as the injection line of

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https://doi.org/10.1016/j.fusengdes.2020.111504
Received 20 September 2019; Received in revised form 20 January 2020; Accepted 22 January 2020

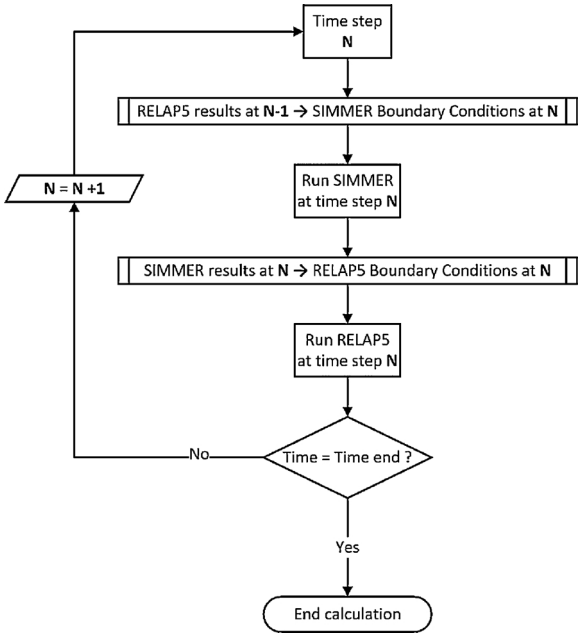

Fig. 1. Flowchart of the explicit time advancement scheme.

LIFUS5/Mod3; secondly because of the extremely high computational effort required and the consequent long calculation time. Therefore, SIMMER-III should be used only to analyse smaller parts of the space domain characterised by an axial-symmetric geometry and in regions where a significant accuracy might be required; on the other hand, the remaining part of the system, mainly composed by 1D components such as pipes, should be simulated with System Thermal-Hydraulic (STH) codes to reduce the computational effort. RELAP5, for instance, is a well-known 1D STH code, extensively used in nuclear applications, particularly suitable for the simulation of complex pipeline systems and able to handle both multiphase flow and changes of phase.

This paper describes the work carried out at the University of Pisa in order to simulate the whole LIFUS5/Mod3 experimental facility through the improvement of a coupling methodology between SIMMER-III and RELAP5/Mod3.3; this methodology was recently validated for liquid single-phase fluids [8]. It is shown here that the coupling technique is also able to handle complex multiphase coupling. In particular, this paper is dedicated to the presentation of this technique, which allows to couple the two codes via multiphase boundary conditions. Through this methodology, it is possible to correctly update and synchronise the two codes and their boundary conditions, even in a complex transient multiphase scenario involving phase transitions. To the authors' knowledge this is the first attempt to develop this kind of coupling.

2. Coupling methodology

The coupling tool between SIMMER and RELAP5 codes, developed at the University of Pisa, can be classified as a "two-way", "non-overlapping" and "online" procedure, since the computational domains of the two codes communicate by separated interfaces (i.e. text files) which are used to exchange data in both directions, with a synchronized progression in time. The interaction is managed by several MATLAB scripts, which also have the role to check the "consistency" of the physical properties exchanged at the interface. An explicit method was chosen as numerical scheme; in this kind of scheme each code performs one independent calculation for each time step and then the coupled variables are exchanged sequentially between the two codes at the end of the time step; in other words, the results obtained in the previous time step from one code are used as new boundary conditions for the other code, which will simulate the next time step [8]. A simplified flowchart of the explicit scheme is shown in Fig. 1

In addition to the basic information exchanged in the liquid single phase coupling (liquid temperature and pressure), in this multiphase coupling the two codes have to share data also on the non-condensable fluid and vapours which compose the gas phase: these data include the gas velocity and the gas mixture temperature.

In order to avoid inconsistencies in the physical properties, this gas-phase coupling was developed as one-way coupling, i.e. the properties of the mixture at the interface are always calculated by SIMMER using data from RELAP5 and no other exchange is done. The scheme for the calculation of the gas mixture properties is shown in Fig. 2: RELAP5 communicates the total pressure (P_{TOT}), the gas temperature (T_{GAS}) and the liquid temperature (T_{LIQ}) to SIMMER which calculates the vapour pressure (P_{VAP}) from T_{LIQ}. Then P_{VAP} is assumed as the partial pressure of the vapour in the gas mixture and the partial pressure of the incondensable gas (P_{INC}) is determined in order to keep P_{TOT} to the imposed value. The final properties of the gas mixture in SIMMER are eventually calculated according to P_{VAP}, P_{INC} and T_{GAS}.

3. LIFUS5/Mod3 facility

LIFUS5/Mod3 is an experimental facility designed and developed at the ENEA Brasimone Research Center (Italy). The aim of the facility is to investigate the physical and chemical interaction of water and PbLi

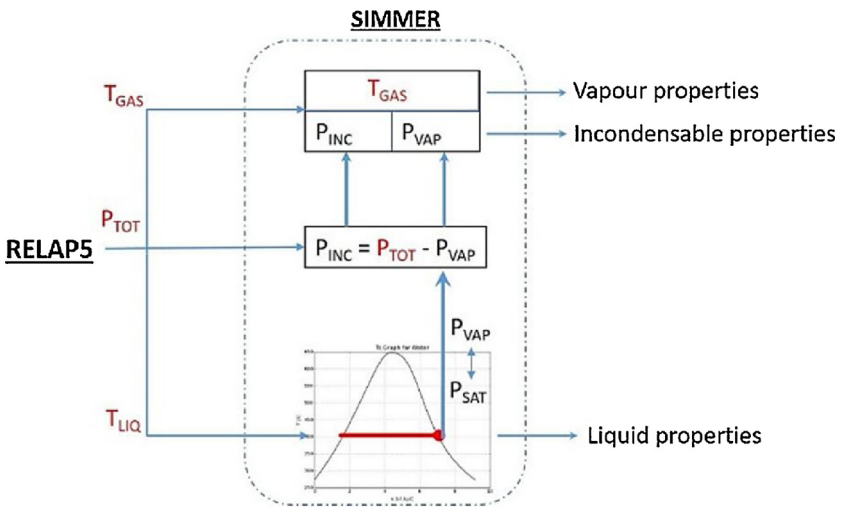

Fig. 2. Gas mixture properties scheme.

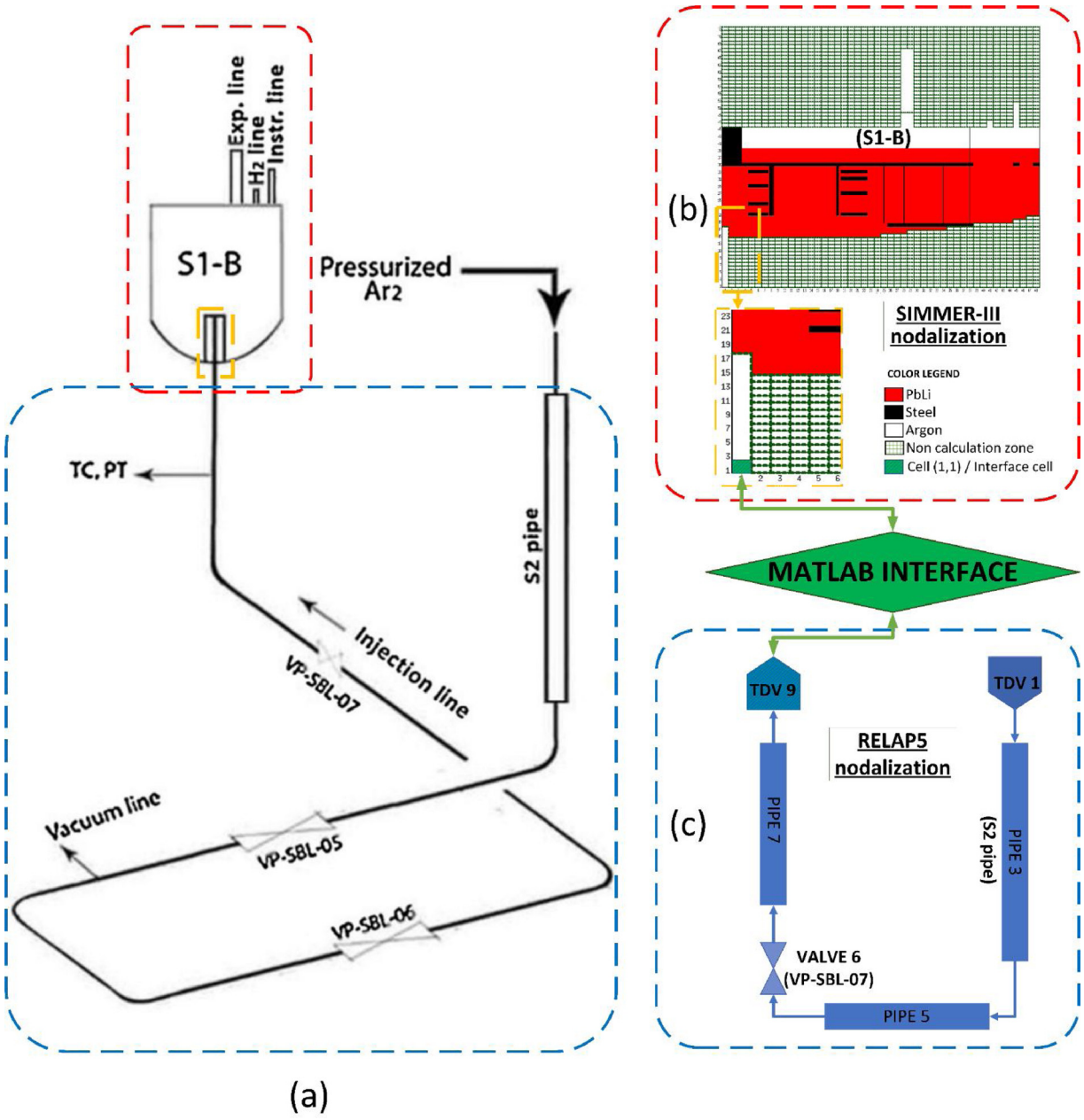

Fig. 3. LIFUS5/Mod3 facility (a) modeled by SIMMER III (b) and RELAP5 (c) coupled codes.

Table 1
Initial conditions of the coupled domains.

Parameter	Design value	Domain
Abs. pressure in S1-B tank (Pa)	10^5	SIMMER
PbLi temperature in S1-B tank (°C)	330	SIMMER
Injected water temperature (°C)	300	RELAP5 (pipe 5)
Injected water mass (g)	~25	RELAP5 (pipe 5)
Ar abs. pressure in injection line (Pa)	0.1×10^5	RELAP5 (pipe 7)
Ar inlet pressure (MPa)	15.5	RELAP5 (TDV 1)

alloy. A simplified scheme of the facility is presented in Fig. 3(a): it consists of an injection line partially filled with water and Argon, and a reaction tank (S1-B) in which the heavy liquid metal is contained. The geometrical volume of the S1-B vessel is about 30 L and during the experiments is filled with Lead-Lithium alloy and covered with Argon at about 0.2 barg. The water injection line penetrates into the S1-B vessel from the bottom, aligned with its axis; in this way an axial-symmetric configuration is obtained, in order to facilitate the nodalization of the domain in the SIMMER-III code [5]. The injection line and the S1-B tank are initially isolated by means of a rupture disk, installed at the exit of the injection line (in the S1-B tank). The tank is initially at atmospheric pressure, while the injection line is at a higher pressure.

One of the main tasks of the LIFUS5/Mod3 experimental campaign is to validate the application of the SIMMER code for the prediction of PbLi-water interaction and to improve and verify the reliability of the coupling methodology between SIMMER-III and RELAP5 presented here [5,7].

4. Application of coupling methodology

4.1. Computational domains

In the coupled simulation, the S1-B vessel and the last part of the injection line are simulated by SIMMER-III, whilst the remainder of the injection line through RELAP5; both nodalizations are shown in Fig. 3.

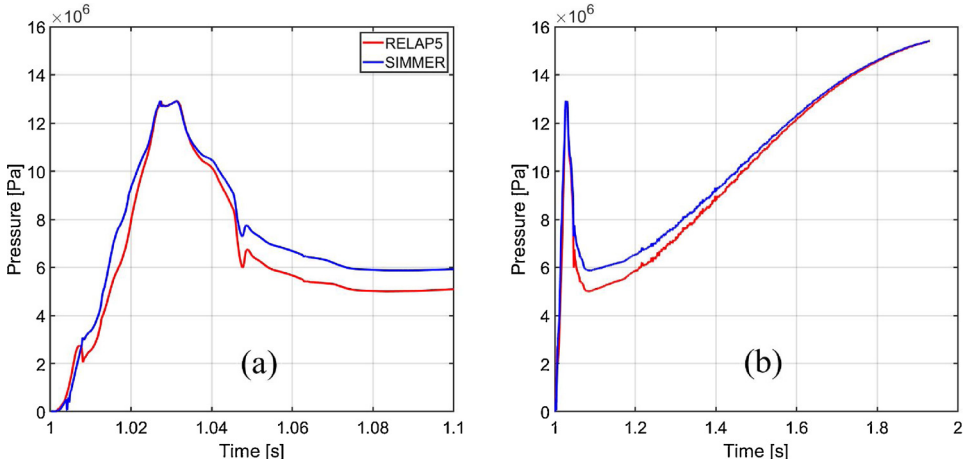

Fig. 4. Time evolution of pressure at the coupled interface and at different time intervals.

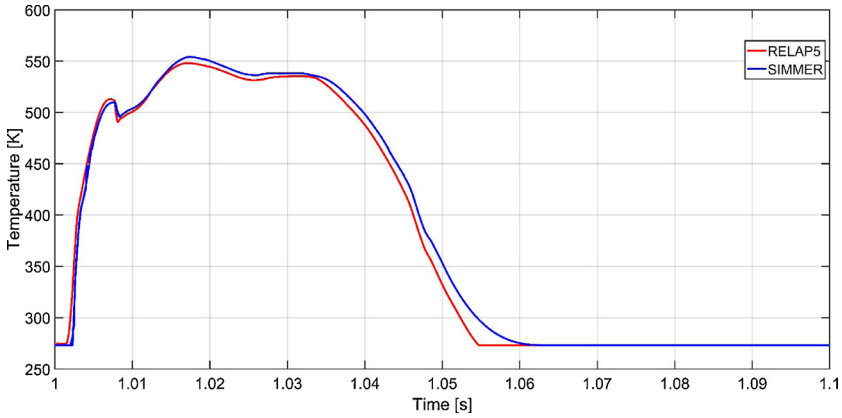

Fig. 5. Time evolution of liquid water temperature at the coupled interface.

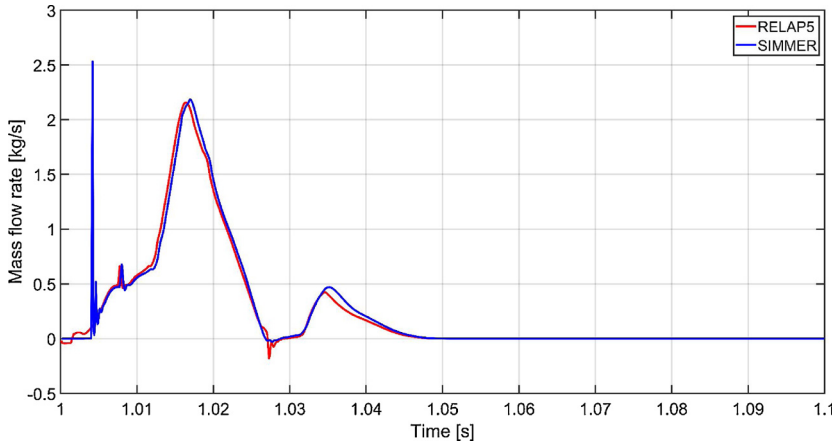

Fig. 6. Time evolution of liquid water flow rate at the coupled interface.

In the SIMMER nodalization an attempt was made to reproduce all the features of the S1-B vessel, namely the expansion line with the rupture disk, the hydrogen discharge line and the instrumentation line, together with the internal structures necessary to support the instrumentation (steel material in Fig. 3(b)). Further details can be found in [7].

The RELAP5 nodalization is shown in Fig. 3(c) and it is composed of two vertical and one horizontal sections (pipes 3, 7 and 5, respectively) which have the same geometrical characteristics of the LIFUS5 pipes. Two Time Dependent Volumes (TDV) are necessary in the nodalization: TDV 1 is used to impose the boundary condition at the inlet (i.e. Argon injection line) and TDV 9 provides the interface with SIMMER. Valve 6 is a motor valve which keeps the line closed until the injection starts (the numbering of the components is an internal sorting of RELAP5 and has no relations with the real facility). It is worth noticing that this computational domain is somewhat simplified, since it does not take into account the presence of the bends in the line; since the main aim of this work is the testing of the multiphase coupling in real case scenarios this can be considered an acceptable simplification.

The two computational domains are coupled through TDV 9 and the

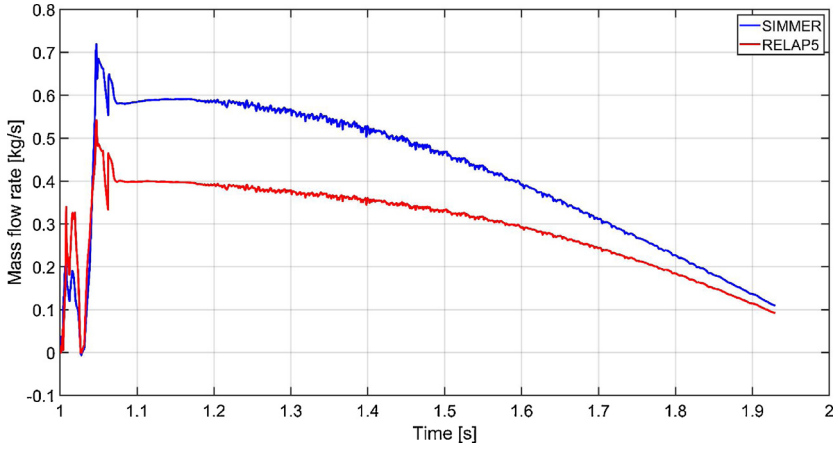

Fig. 7. Time evolution of gas flow rate at the coupled interface.

boundary at the bottom side of cell (1,1) in RELAP5 and SIMMER respectively.

4.2. Test conditions

The initial conditions of the domains are summarised in Table 1.

5. Results and discussion

Since this work is devoted to the development of a coupling technique between two significantly different codes in a complex multiphase scenario, which involves the exchange and the calculation of the properties and thermodynamic state of a mixture of water in liquid and vapour phase and an incondensable gas (Argon), the very first aim must be to obtain a close match between the thermodynamic variables calculated in the cells at the interface of the two domains. Therefore, to evaluate the performance of the coupling methodology, the pressure, liquid temperature and mass flow rate of the liquid water were monitored in the first cell of the SIMMER domain, i.e. cell (1,1), and in the last cell of the RELAP5 domain (namely the last cell of the pipe 7). The predicted time transients are shown from Figs. 4–7 and discussed below.

Valve 6 is set to open after 1 s, therefore the whole system stays at rest until the pressurisation starts, and so the time axis in all the figures starts at 1 s. In the initial phase of the transient the pressure in the injection line rises steadily, whilst a mixture of Argon and water (in both liquid and vapour phase) begins entering in the S1-B injection section (i.e. the SIMMER domain). The mass flow of liquid through the coupling interface reaches a peak and then decreases down to zero; in this phase, before the injection, around 90 % of the liquid water moves from the RELAP5 domain to the SIMMER domain.

Once the rupture threshold pressure is reached (155 bar), the cap breaks ($t \simeq 1.03$ s) and the S1-B vessel is connected with the injection line. After the rupture of the cap, the mass flow rate of the liquid water increases rapidly until the remaining liquid water is injected and the pressure shows a steep decrease. The pressure keeps diminishing until it reaches a minimum, after which the system starts pressurising again.

Fig. 4 shows that the pressure trend is properly coupled both qualitatively and quantitatively, with only a small offset between the two codes. This offset becomes larger when the liquid water injected becomes very low, after around 1.04 s (Fig. 4a) and it is reduced again towards the end of the transient (Fig. 4b). The reasons of this difference are still under investigation but it is likely due to a discrepancy in the calculation of the gas properties, which consequently causes an inconsistency in the coupled gas flow rate (Fig. 7). Indeed, a more significant difference is present for the mass flow rate of the incondensable gas (Fig. 7). However, since the transient is well captured and pressure and temperature do match in the interface cells, the authors believe that this discrepancy should only depend by the different correlations employed to calculate the Argon density, which are different for the two codes, and it is not due to errors in the coupling methodology. Further investigations are ongoing to better understand this behaviour.

The same good results are shown for the liquid temperature (Fig. 5) and the liquid water mass flow rate (Fig. 6). The latter shows an initial tuning (strong oscillations at around 1.004 s) on the SIMMER side at the very beginning of the coupling stage; this is due to the fact that, in SIMMER, it is not possible to impose the liquid fraction of the water and therefore the code needs to initially adjust the amount of liquid inside the first cell to match the thermodynamic properties imposed by RELAP5.

6. Conclusions

Recently, the University of Pisa developed an original coupling technique between the SIMMER III and RELAP5/Mod3.3 codes, using MATLAB as an interface among the two codes. On the one hand SIMMER III is apt to simulate 2D axis symmetric domains and it is particularly fitted for the analysis of water and PbLi interaction, whilst on the other hand RELAP5 code is suitable for the simulation of composite pipe systems as 1D geometry and hence it can reduce the computational effort of the complete simulation.

An improvement of this technique was presented here, which allows to couple the two codes also for multiphase boundaries. The new improved coupling was applied to the nodalization of a real experimental facility, namely the LIFUS5/Mod3, realized at ENEA Brasimone R.C. (Italy). In the calculation, the chemical reaction between PbLi and water was also considered. The coupling method correctly simulated the transient of all the main properties of the system.

As a result, this coupling tool can provide a high accuracy in calculations involving complex geometries and physical phenomena, such as multiphase flows in experimental loop facilities involving chemical reactions, at a relatively low computational cost.

As further development, a thorough validation of the results against LIFUS5 experimental data is planned in the near future, after the experimental tests will be completed.

CRediT authorship contribution statement

Francesco Galleni: Methodology, Investigation, Writing - original draft, Writing - review & editing. **Samad Moghanaki:** Methodology, Writing - review & editing. **Marica Eboli:** Writing - review & editing. **Alessandro Del Nevo:** Writing - review & editing. **Sandro Paci:** Writing - review & editing. **Riccardo Ciolini:** Writing - review & editing. **Rosa Lo Frano:** Writing - review & editing. **Nicola Forgione:**

Supervision, Writing - review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

With reference to the part of the work concerning the development of the coupling technique between RELAP5 and SIMMER, the authors acknowledge the funding “Progetti di Ricerca di Ateneo (PRA) 2018-2019” received from the University of Pisa.

References

[1] L.V. Boccaccini, et al., Objectives and status of EUROfusion DEMO blanket studies, Fusion Eng. Des. 109–111 (2016) 1199–1206, https://doi.org/10.1016/j.fusengdes.2015.12.054.

[2] A. Del Nevo, et al., WCLL breeding blanket design and integration for DEMO 2015: status and perspectives, Fusion Eng. Des. 124 (2017) 682–686, https://doi.org/10.1016/j.fusengdes.2017.03.020.

[3] E. Martelli, et al., Advancements in DEMO WCLL breeding blanket design and integration, Int. J. Energy Res. 42 (2017) 27–52, https://doi.org/10.1002/er.3750.

[4] M. Eboli, et al., Implementation of the chemical PbLi/water reaction in the SIMMER code, Fusion Eng. Des. 109–111 (2016) 468–473, https://doi.org/10.1016/j.fusengdes.2016.02.080.

[5] M. Eboli, et al., Experimental activities for in-box LOCA of WCLL BB in LIFUS5/Mod3 facility, Fusion Eng. Des. 146 (2019) 914–919, https://doi.org/10.1016/j.fusengdes.2019.01.113.

[6] M. Eboli, et al., Test Series D experimental results for SIMMER code validation of WCLL BB in-box LOCA in LIFUS5/Mod3 facility, 14th International Symposium on Fusion Nuclear Technologies, Budapest (Hungary), 2019.

[7] S.K. Moghanaki, et al., Validation of SIMMER-III code for in-box LOCA of WCLL BB: Pre-test numerical analysis of Test D1.1 in LIFUS5/Mod3 facility, Fusion Eng. Des. 146 (2019) 978–982, https://doi.org/10.1016/j.fusengdes.2019.01.131.

[8] B. Gonfiotti, et al., Development of a SIMMER\RELAP5 coupling tool, Fusion Eng. Des. 146 (2019) 1993–1997, https://doi.org/10.1016/j.fusengdes.2019.03.084.