HYDROGEN DEFLAGRATION ANALYSES IN THAI EXPERIMENTS USING MELCOR CODE

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ABSTRACT

In order to develop an appropriate knowledge to support the SUJB (State Office of Nuclear Safety), the CVŘ (Research Centre Řež), in collaboration with SURO (National Radiation Protection Institute) is developing a methodology to simulate nuclear power plants under accidental conditions. A particular effort is focused in the severe accident phenomenology where hydrogen deflagration carries a critical issue for the containment integrity, such as Fukushima Daiichi accident. For this purpose, THAI (Thermal-hydraulics, hydrogen, aerosol and iodine) experimental campaigns are chosen due to the several tests involved in different conditions. THAI containment test facility is used to open questions concerning the behaviour of hydrogen, iodine and aerosols in the containment of water-cooled reactors during severe accidents.

The Fukushima Daiichi Accident demonstrates that the hydrogen deflagration could lead to a significant containment damage. For this reason, a particular attention is given to the hydrogen deflagration scenario. All simulations are prepared and modelled in MELCOR 2.1.

The results obtained showed a strong influence related with some factors as: the nodalization pattern, control volume number CV, flow paths number FP and time step. In order to assess the THAI model with the THAI final reports, a sensitivity analysis focused with those parameters was performed.

KEYWORDS
Severe Accidents, MELCOR, Hydrogen Deflagration, Modelling & Simulation.

1. INTRODUCTION

After Fukushima Daiichi Nuclear Power Plant (NPP) accident, the European Commission required to carry out stress tests on all NPPs placed in the European Union (EU) member states. The conclusions of this analysis have led EU members to improve their knowledge on severe accident phenomenology. In Czech Republic, this occurred by the State Office of Nuclear Safety (SUJB), which has set up a consortium of research organizations and universities (SURO v.v.i., Research Centre Řež s.r.o., SUJCHBO v.v.i. and ČVUT FJFI) [1]. The CVŘ in collaboration with SURO, is working to increase the capability to analyse Beyond Design Basic Accidents (BDBAs), focusing on phenomena as core melt accident, behaviour of containment building, hydrogen production, deflagration, production and release of radionuclides.

During a severe accident scenario, the hydrogen combustion can occur and lead to containment integrity failure, since it generates local and global pressure and heat spike. Therefore, theoretical analyses are needed, in order to obtain a reliable prediction of the accidental scenario. This work aims to assess the capability of CVŘ and SURO to simulate hydrogen deflagration scenario in the containment of NNPs, increasing the level of confidence in nuclear reactor containment safety research. For this reason, it was decided to simulate one of the hydrogen deflagration experiment performed in THAI containment test facility. THAI is a German facility, built for experimental research in NPPs containment safety. The facility allows to investigate safety relevant effects under thermal-hydraulics conditions of severe accidents. The scenario simulated, range from hydrogen deflagration to iodine and aerosol behaviours [6].

In the initial step for this study, the 24th Hydrogen Deflagration experiment (HD-24) has been chosen (24th out of 29 HD experiments) [4]. In the HD-24 experiment, the vessel is filled with homogeneous air-steam-hydrogen mixture and the ignitor is placed in the bottom part of the vessel so that upward flame propagation should occur. Such initial condition allows to create a consistent set of models pointing out the MELCOR code limitations. In particular, the simulation of the flame front propagation is done using a parametric and isotropic approach inside the BUR package. After that, the experiment has been modelled in four ways by varying the nodalization pattern. Two out of four models were discretized by the intersection of several vertical and horizontal planes, while the other two have a toroidal nodalization pattern. The models have been created, ranging from a rough model with 7 Control Volumes (CVs) and 13 Flow Paths (FPs) to a much more refined one with 119 CVs and 351 FPs. Finally, the results of calculation have been compared with the experimental results in order to point out the influence of the nodalization.

2. THAI TEST FACILITY

2.1. Basic Configuration

THAI, which stands for Thermal-hydraulics, Hydrogen, Aerosols, Iodine is a containment test facility which is operated by Becker Technologies GmbH at Eschborn, Germany. The main component of the facility is a cylindrical stainless-steel vessel of 9.2 m height, 3.2 m diameter and total volume of 60 m^3. The THAI vessel wall (in the cylindrical part) is double-walled and the gap between the walls (16.5 mm) is filled with thermal oil of the wall heating/cooling system. Two dished heads of 30 mm diameter form bottom and top part of the vessel both of which are penetrated in the vessel axis by cylinders. The upper cylinder carries a 120 mm thick top flange; the lower cylinder is closed by a 16 mm thick dished head. The vessel is designed to withstand 1.4 MPa of pressure at 726.3 K and its size allows to study heat and mass transport processes in large-scale (even multi-compartment) geometry through a natural convection flow [5] [6].

HD-tests (Hydrogen Deflagration-test) have been performed in the THAI vessel in which the inner cylinder and condensate trays have been removed. Figure 1 shows the vessel configuration for HD-tests [5] [6].

2.2. HD-24 test configuration

The THAI test HD-24 consist of experiment involving homogeneous H_2-steam-air mixtures at superheated and saturated conditions. This test has been performed with upward burn direction (initiated by vessel bottom ignition), initial pressure of 0.15 MPa and elevated initial temperature. Moreover steam (48.2 vol%) has been added to the initial gas mixture (0.71 bar saturation pressure is related to 363.45 K). Initial test conditions are listed in Table I [5] [6].

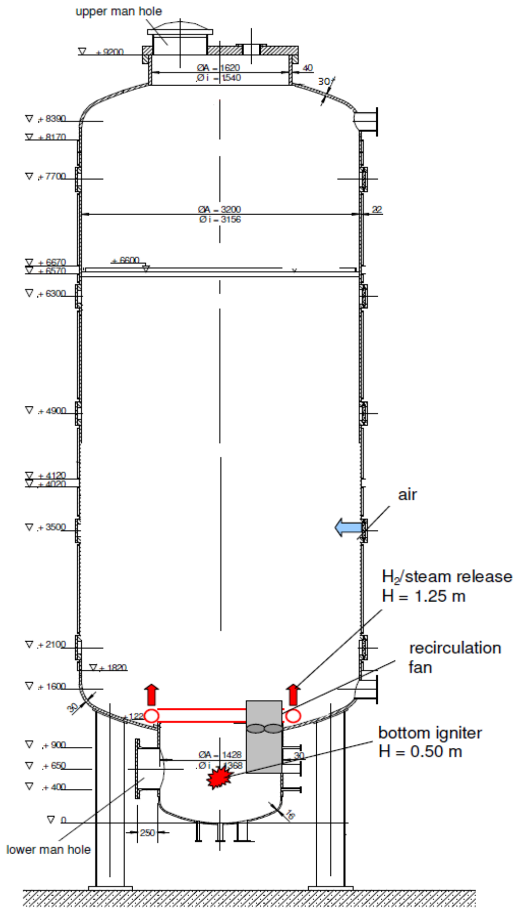

Figure 1. THAI facility [5] [6]

Table I. The initial parameters of HD-24 test [5] [6]

	Test parameters	
	specified	**measured**
p [MPa]	0.15	0.1472
T [K]	363.15	363.45
H_2 [vol%]	10	9.79

3. CODE DESCRIPTION

The MELCOR code is a fully integrated, system computer code which allows to model the progression of severe accidents in light water nuclear power plants. This code is developed by Sandia National Laboratories for the needs of the U.S. (United States) Nuclear Regulatory Commission. MELCOR is used to perform sensitivity and uncertainty analyses in different applications [4].

The severe accident simulations involve a broad range of phenomena, including thermal-hydraulic feedback in the reactor coolant system and containment; the core overheating, its degradations and the gradual relocation in the bottom of the vessel; the hydrogen production and the fission products issue [4].

Thermal-hydraulic behaviour of water and gases in MELCOR are modelled by control volumes and flow path packages. The control volumes include so-called hydrodynamic materials (associated with their energy), such as the water, the vapor, the fog and the non-condensable gases. The flow paths are the connections between the control volumes through which the hydrodynamic materials can flow. Each connection is referred to two junctions, which can be at different elevations. Since material cannot reside in flow paths, there is no heat and mass transfer between hydrodynamic materials [4].

The hydrogen combustion is handled by the burn package model. The burn model implemented takes into account the effects of burning premixed gasses without tracking the flame front propagation. The deflagration is ignited if the mole fraction composition in the control volume meets the LeChatelier's criterion. Due to the flow path, deflagration can propagate into the adjoined control volumes. The combustion rate is given by the flame speed, the volume characteristic dimension and the combustion completeness [4].

4. THAI FACILITY MODELS IN MELCOR CODE

In lumped parameter approach, it is important to create a nodalization which allows to cope with the limitations of the method. In particular, this study is aimed to understand how the user effect impact can be reduced on calculation results. The THAI facility has been modelled in four different ways in order to point out the influence of nodalization. Each model differs from the others in nodalization pattern, CV number and Flow Paths (FP) [2] [3].

Two out of four models have toroidal nodalization, while the others two have CVs obtained by the intersection of several vertical and horizontal planes. Firstly, the model A was developed and it consists of 7 CVs connected by 13 FPs, as it is shown in Figure 2 A). This simple nodalization is obtained by the intersection of several vertical and horizontal planes. Afterward, a more detailed mesh is implemented to create the model B, shown in Figure 2 B). In this case, the mesh pattern is the same as the model A and it is obtained by connecting 97 CVs with 180 FPs. The model C (see Figure 2 C), has 97 CVs connected with 214 FPs. In the main cylinder body (from 1.60 m to 8.17 m), the discretization pattern consists of hollow or solid half cylinders with the same diameter. Finally, the most refined model D (see Figure 2 D) that has 119 CVs connected with 351 FPs was developed. In this case, the discretization has conical pattern and consists of cylindrical bodies, which have diameters that vary depending on the facility height. As it possible to see in the Figure 2, the red arrows represent the radial and the vertical flow paths.

The initial and boundary conditions, as atmosphere composition, quality, initial pressure, initial temperature and the ignitor position, are taken from THAI final report [5]. At time 0 second, the whole vessel is filled with homogeneous H_2-steam-air mixtures at superheated and saturated. The volumetric atmosphere concentrations evaluated by Dalton's law of partial pressures, are 10% H_2, 18.9% O_2 and 71.1% N_2. The initial pressure is 0.147 MPa and the temperature is 363.45 K [5].

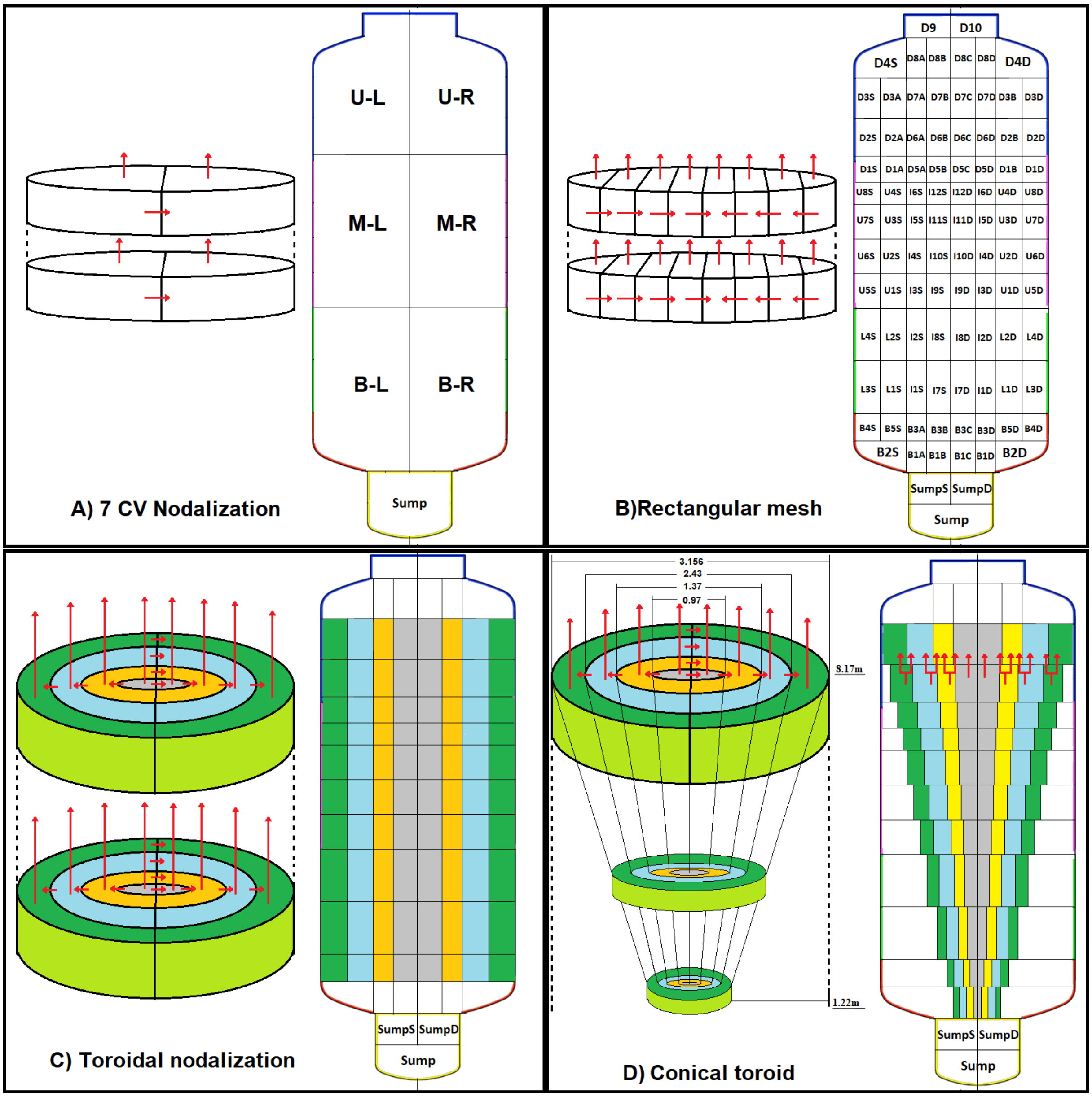

Figure 2. Nodalization Patterns.

5. RESULTS

The results achieved have been compared with the measurements done during the experiment. In particular, the plots point out the pressure and temperature trends at elevations 4.9 m and 7.7 m. The first plots, Figure 3 and Figure 4, shown the pressure trend as function of time. In both vessel elevations, the pressure peak is well predicted by the B, C and D model. Whereas, the model with 7 control volumes highlights a slight decrease of the peak pressure. Each pressure profile calculated is steeper than the experimental one. This happens because the burn models, implemented in MELCOR code, consider the effects of burning premixed gases without modelling the actual reaction kinetics or tracking the actual flame front propagation [4].

Figure 5 shows that, the model B, C and D predict the experimental temperature peak, but not the trends. At 7.7 m elevation, neither the peak nor the trend are predicted by any model as shown in Figure 6 [2] [3].

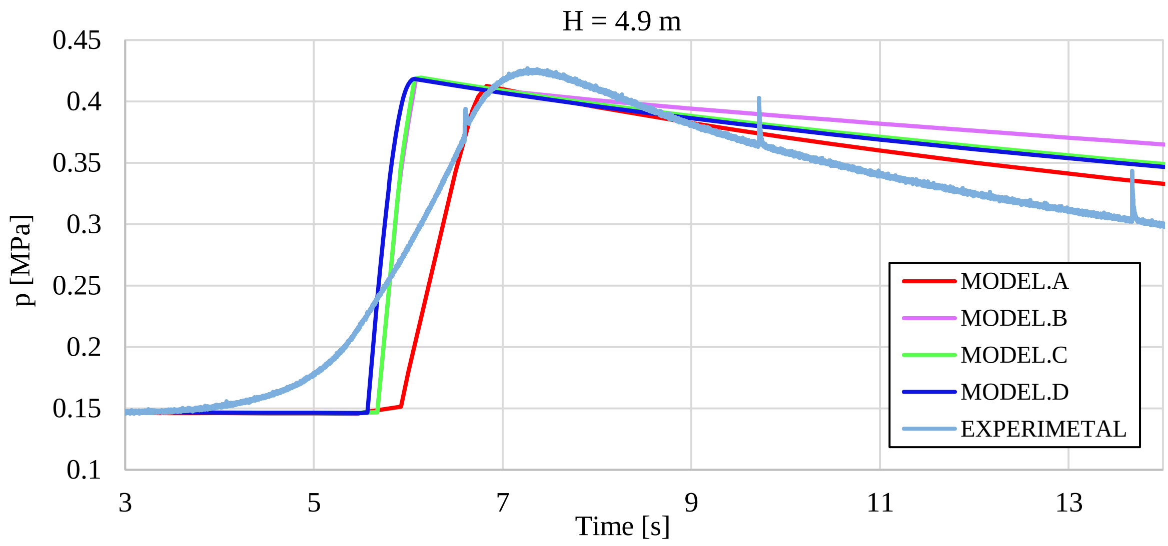

Figure 3. Pressure vs. Time at 4.9 m

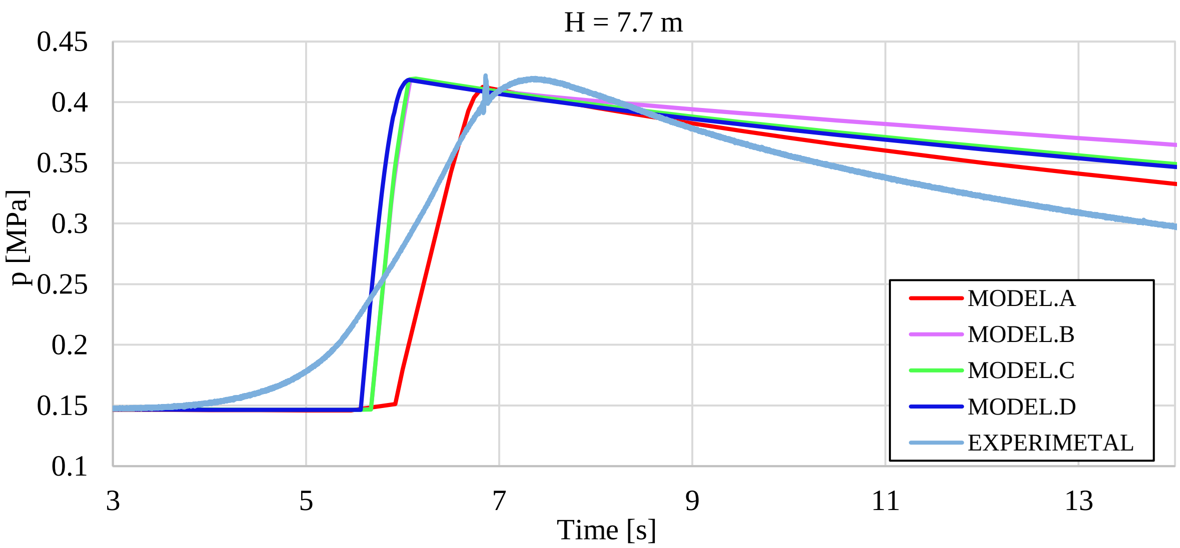

Figure 4. Pressure vs. Time at 7.7 m

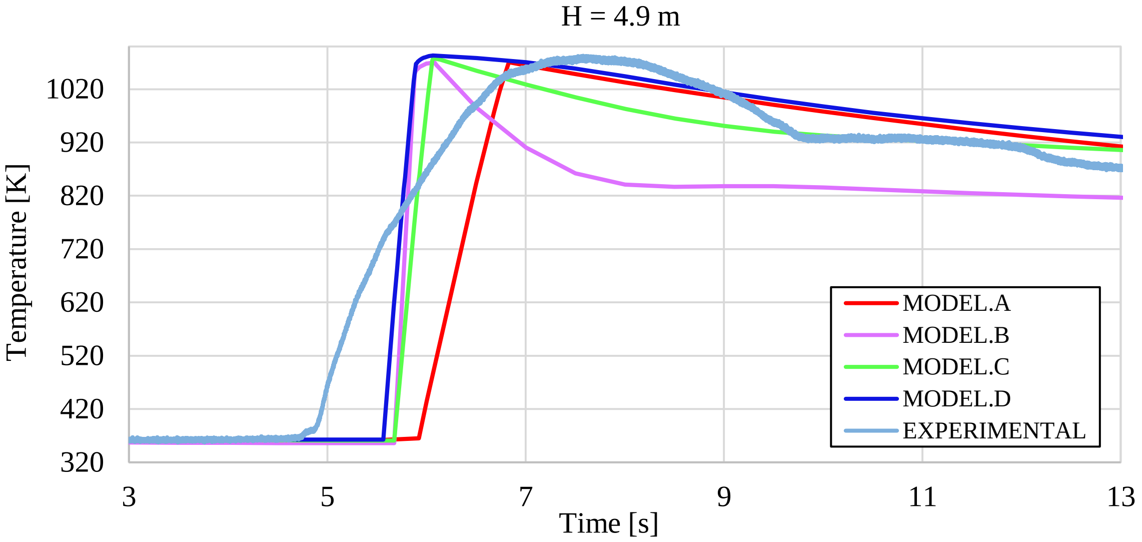

Figure 5. Temperature vs. Time at 4.9 m

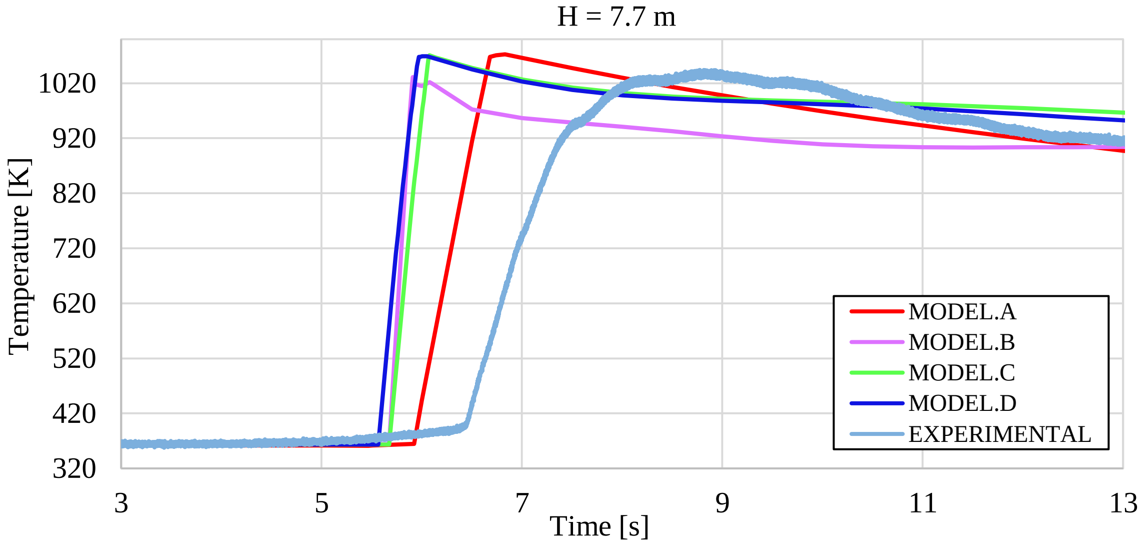

Figure 6. Temperature vs. Time at 7.7 m

Figure 7, Figure 8, Figure 9 and Figure 10 show the flame propagation in the different modelling approach through the hydrogen reaction rate. For each model, 3 different times were selected:

1. 5.46 s is the time when the ignition control function in the BUR package start the hydrogen deflagration.
2. 5.94 s (Model A) and 5.66 s (Models B, C and D) represent the maximum reaction rate gradient for each model, and
3. when the maximum pressure peak for each model is reached (just the instant before when the flame shutdown)

In the case of the models B, C, and D the deflagration starts in the CV immediately above the ignitor; the nodalization mesh distributions influence the reaction rate values with a maximum for the model B (0.005521 kg/s) and a minimum value for model D (0.001196 kg/s). When the deflagration rises its maximum, (at 5.66 s for models B, C, D and 5.94 for model A), each model is characterized by its own peculiarity simulation. Due to the simplification in the number of CVs, model A appears to have the symmetrical progression. In the case of model B, the reaction rates evidenced a higher rate in the central CVs in comparison with the peripherical CVs. In the model C and D, the flames seem propagate on the external CVs with different reaction rate gradient: the model C has higher hydrogen rate in the central element than the model D that appears already exhausted. Finally, in analogy for each model the extinguish time comes at the approaching of the maximum pressure peak with a gradient based on the hydrogen burn rate distribution.

Table II points out the difference between the results as function of models features and the difference among the models' prediction and the experimental measurements. Each model has given a pressure peak which differs from the experimental one by 3.35%, in case of model A and by 1.73% in case of model D. Regarding the maximum temperatures calculated, the difference between the computational and experimental results is by up to 28.7 K. Clearly, the results calculated by the model A show the biggest difference with the ones measured during the experiment. As it might have been expected, the computational time increases with increasing CVs.

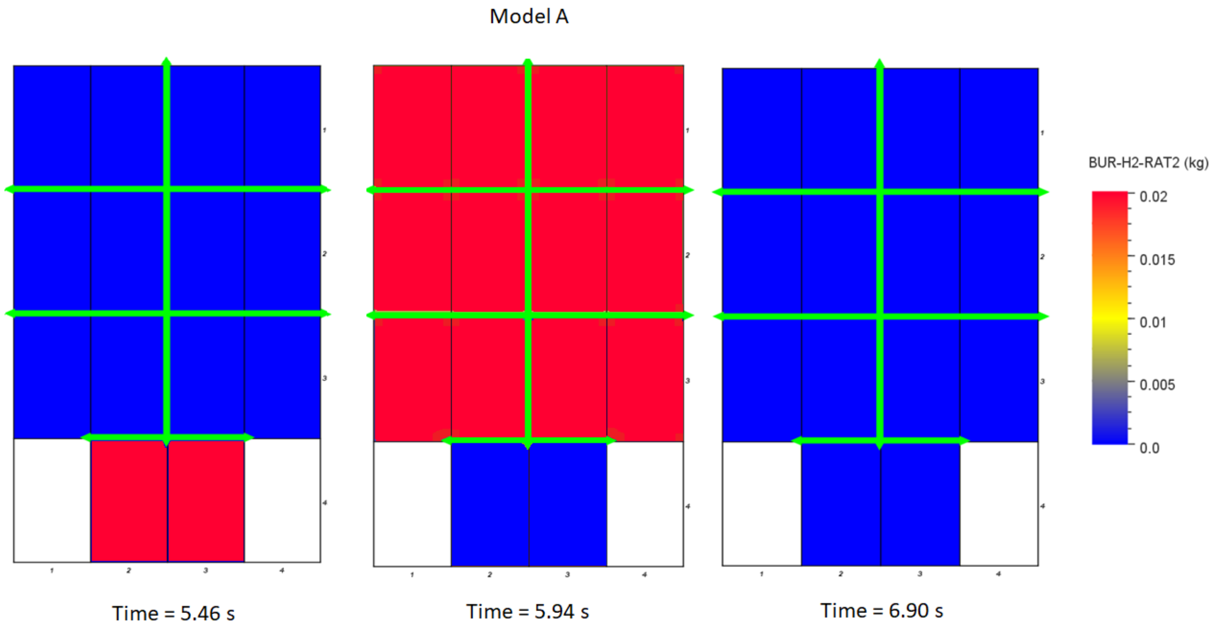

Figure 7. Model A. H_2 Reaction rate.

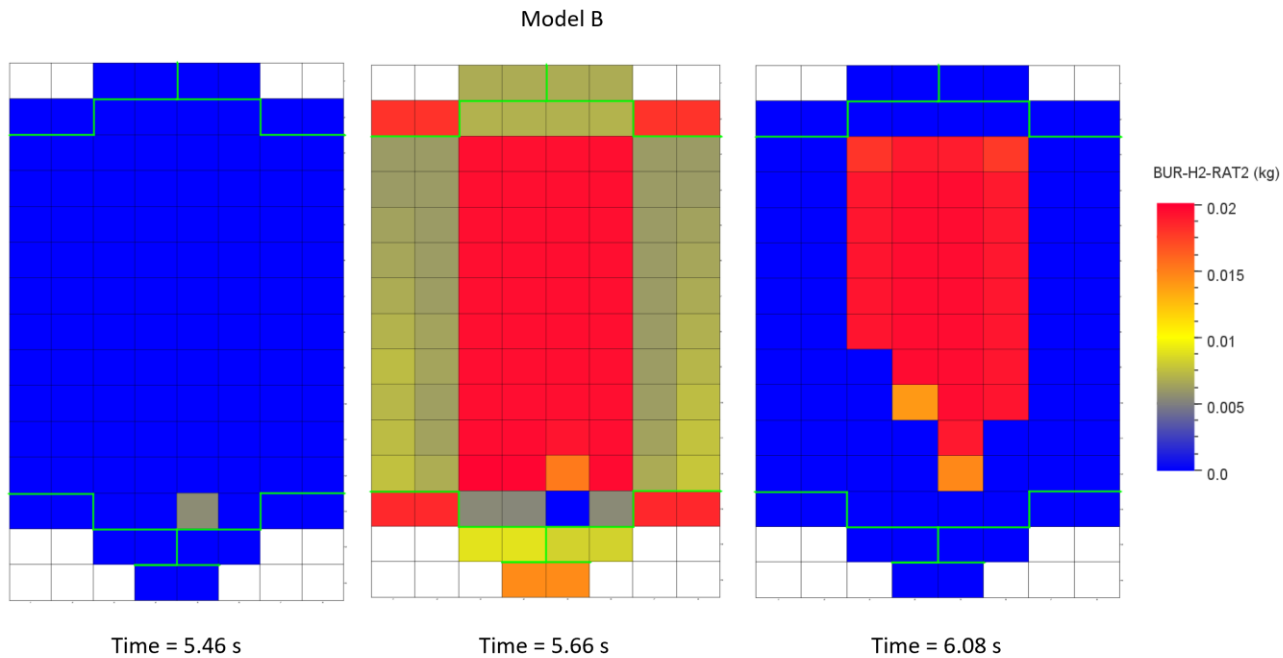

Figure 8. Model B. H_2 Reaction rate.

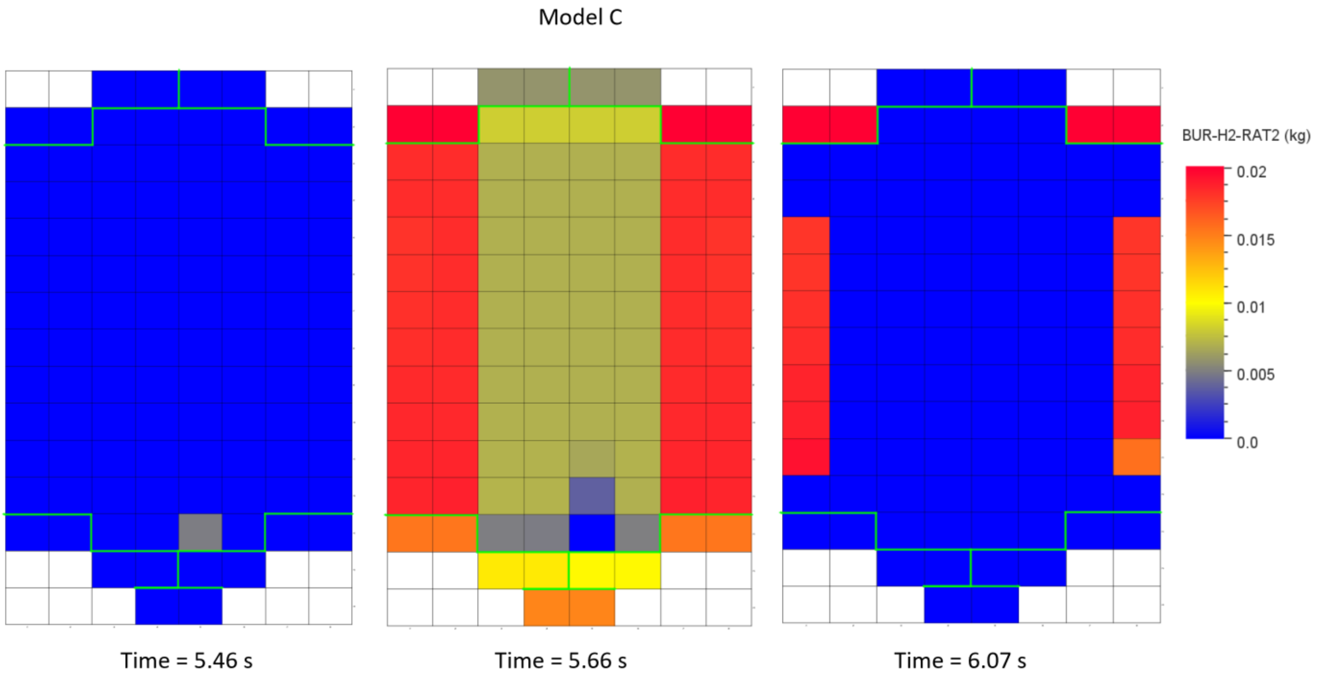

Figure 9. Model C. H_2 Reaction rate.

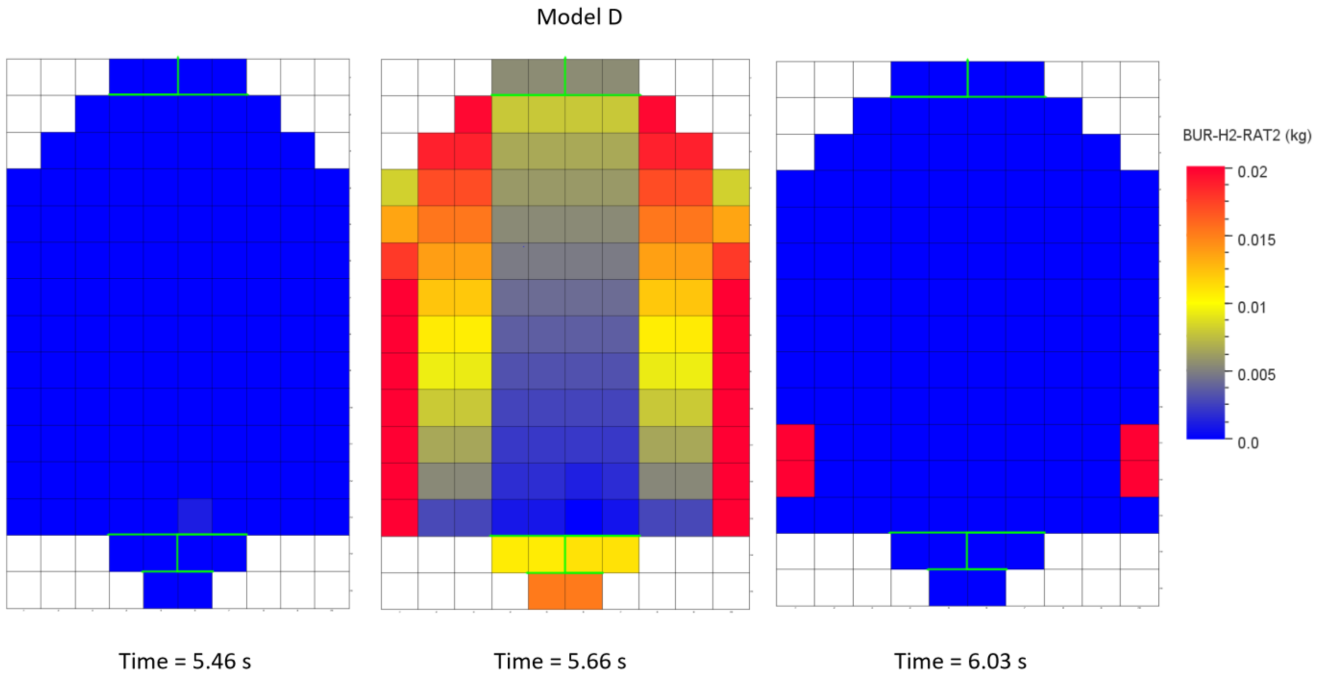

Figure 10. Model D. H_2 Reaction rate.

Table II. Calculation results

Model	CV	FL	p_{max} [MPa] / Time [s]	T_{max} [K] / Time [s]	Computational time [h]	$\left\lvert\frac{p_{ext} - p_{mod}}{p_{ext}}\right\rvert$ [%]	$\left\lvert\frac{T_{ext} - T_{mod}}{T_{ext}}\right\rvert$ [%]
A (4.9 m)	7	13	0.4126	1070.57	~1	3.35	1.12
			6.83	6.83			
A (7.7 m)			0.4125	1072.61		1.79	2.75
			6.83	6.83			
B (4.9 m)	97	180	0.4182	1070.03	~9	2.04	1.17
			6.08	6.07			
B (7.7 m)			0.4182	1030.94		0.43	1.25
			6.08	5.91			
C (4.9 m)	97	214	0.4184	1082.83	~9	1.99	0.0074
			6.06	6.06			
C (7.7 m)			0.4184	1069.19		0.38	2.42
			6.06	6.04			
D (4.9 m)	119	351	0.4195	1077.94	~18	1.73	0.44
			6.14	6.08			
D (7.7 m)			0.4195	1070.891		0.12	2.58
			6.08	6.08			
EXP (4.9 m)	-	-	0.4269	1082.75	-	0.0	0.0
			7.26	7.58			
EXP (7.7 m)			0.42	1043.95		0.0	0.0
			7.34	8.77			

6. CONCLUSIONS

The main purpose of this work was achieved by creating the computational models of THAI-HD and performing a sensitivity analysis. The results of this study present a quantitative overview of our capability to simulate the hydrogen deflagration scenario using the MELCOR code.

The simulations of HD-24 THAI experiment (upward flame propagation) have shown that MELCOR code can predict the pressure peak generated during deflagration scenario [5]. Each pressure peak calculated by simulations, is slightly lower than the experimental one. By increasing the number of CVs is possible to reduce the difference between the experimental peak pressure and the calculated one. Unfortunately, a refined mesh does not allow to calculate the pressure growth rate shown by the measurement during the THAI experimental campaign. This is due to the burn models implemented in

MELCOR code, which consider the effects of burning premixed gases without modelling the actual reaction kinetics or tracking the actual flame front propagation and the speed of combustion process itself [2] [3].

This study shows the MELCOR capability to evaluate the value of overpressure during hydrogen deflagration scenario. This allows to assess the containment integrity during severe accident condition. Furthermore, this goal can be achieved with a coarse nodalization, in order to reduce the computational time.

MELCOR is not suitable for an accurate study of hydrogen deflagration and the results obtained are not strongly influenced by the nodalization, except the flame propagation where the nodalizaion and the way that the CVs are connected played an important role in the hydrogen reaction rate results. The next steps are going to be the hydrogen deflagration test with other boundary conditions, such as downward front propagation and stratified containment atmosphere and to assessment of passive autocatalytic recombiners [2] [3].

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