HYDROGEN DEFLAGRATION SIMULATIONS WITH THE ASTEC CODE

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This paper presents the modeling of the slow hydrogen deflagration tests HD-22 and HD-23 carried out in the THAI experimental facility with the flame FRONT model (the latest version) of the CPA containment module of the ASTEC code. The calculations were performed assuming an exponential burning profile in time as well as a linear burning profile. The simulation results of flame front propagation are compared to experimental data.

Keywords: flame front, severe accident, slow deflagration

1. Introduction

During a severe accident at a nuclear power plant, large amounts of hydrogen can be released. Combustion of the resulting hydrogen-air-steam mixtures could lead to the thermal and mechanical loads that may threaten the integrity of the containment. The state-of-the-art mitigation systems can reduce significantly the hydrogen hazards in different severe accident scenarios. However, even if such mitigation systems are installed in the reactor containment, hydrogen combustion at relatively low concentrations may occur.

To investigate the phenomena of hydrogen combustion, experiments are being performed in various experimental facilities. One of these is the THAI containment test facility located at Eschborn, Germany [1].

The general objective of the hydrogen deflagration experiments in this facility, performed in the frame of the OECD-THAI project, was to investigate hydrogen deflagrations at low concentrations with vertical flame propagation in a sufficiently large geometry under conditions typically for severe accidents [2]. Apart from the contribution to an improved understanding of hydrogen combustion phenomena, the data generated in the experimental program have been used to validate and improve Lumped Parameter and CFD codes available and under development for containment analysis [2]. The hydrogen deflagration tests HD-22 and HD-23 were used to study the flame front propagation in upward and downward direction respectively, in premixed air-steam-hydrogen atmosphere at superheated conditions and elevated initial temperature and pressure. These

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tests were selected for the 'blind' phase of the OECD/NEA International Standard Problem on hydrogen combustion ISP-49 (HD-23 for optional calculations) [3].

This paper presents the modeling of the slow hydrogen deflagration tests HD-22 and HD-23 with the flame FRONT model within the CPA containment module of ASTECv2.0.

The model calculates the propagation of the hydrogen combustion from one containment room into adjacent ones. The calculation of the hydrogen deflagration velocity in the junctions and of the burning rates inside the respective zones is based on several empirical correlations, which include empirical constants. Two sets of default values and uncertainty ranges (for the exponential and linear burning profiles in time) for the model input (empirical) parameters were determined as a result of an extensive parametric study performed with the latest version of the model on six different hydrogen combustion experiments covering a broad range of geometries and scenarios [6].

The aim of this paper is to investigate the influence of the variation of the input parameters for the flame front model with respect to the deflagration velocity, the pressure and the temperature in the experimental vessel. Also, these two tests were calculated with the new sets of default parameters for the flame front model. The calculations were carried out with ASTECv2.0r3p2.

2. Experiments

Main component of the THAI facility is a cylindrical stainless steel vessel of 9.2 m height and 3.2 m diameter, with a total volume of 60 m^3. The cylindrical part of the test vessel is equipped with three independent heating/cooling jackets over the height with external thermal oil circuits. The outer sides of the vessel and the heating/cooling jackets are thermally insulated by rock wool [4].

The hydrogen deflagration tests HD-22 and HD-23 were carried out in the THAI vessel without any internal structures. The test facility has been equipped with the gas and steam feeding devices, a recirculation fan and the igniters. The vessel was filled homogeneously with the hydrogen-air-steam mixture which was ignited at the bottom for the HD-22 test and at the top for the HD-23 test.

The HD-22 test with upward flame propagation was performed at an initial temperature of 91.9°C and an initial pressure of 1.487bar. The initial atmospheric composition was: hydrogen concentration 9.9% vol., steam concentration 25.3% vol. The measured values of the initial conditions for the HD-23 test with downward flame propagation were: pressure 1.465bar, temperature 91.2°C, steam concentration 25.3 % vol. and hydrogen concentration 11.95 % vol.

3. Flame FRONT model

The FRONT combustion model of the ASTECv2.0 code calculates the flame front velocity resulting in the tracking of the propagation of the flame between different containment compartments. In FRONT, the flame propagation is modeled inside the junctions. The H_2 combustion takes place in the zones. The burning velocity inside the zones is determined by the flame front velocity calculated by FRONT.

The calculation of the hydrogen deflagration velocity is based on empirical correlations. The turbulent flame front velocity V_t is calculated with the Peters correlation [3]. This correlation is a function of the laminar flame front speed, the maximal eddy length in the junction $\boldsymbol{l}$, the laminar flame thickness l_f that follows from the molecular diffusion coefficient $D = l_f V_l$ and, the turbulence intensity. The laminar flame front velocity is calculated with the Liu-McFarlane correlation [3], depending on the initial pressure, temperature and composition of the mixture. In the FRONT model, the turbulence intensity u' is given by the following correlation based on Reynolds number [3]:

$$u' = CV_g \,\mathrm{Re}^n \tag{1}$$

with C and n constants with values estimated based on small scaled experiments. V_g is the gas velocity in the junction and Re the Reynolds number. The flame front velocity that describes the propagation of the flame is calculated as the sum of the gas velocity in the junction, V_g and the flame velocity in the junction V_t **:**

$$V_{flame} = \sigma V_t + V_g \tag{2}$$

with σ the expansion factor.

Combustion stops according to a correlation derived from THAI HD experiments with-out steam [5]:

$$\chi_{H_2,end} = \chi_{H_2,start}\left[0.5\tanh\left(6.0 - \chi_{H_2,start}\right) + 0.5\right] \tag{3}$$

with $\chi_{H_2,start} / \chi_{H_2,end}$ the volumetric fraction of H_2 where the combustion process start/ends.

4. Experiment simulation

The parameter study [6] performed with the latest version of the FRONT model on six different hydrogen combustion experiments, with a broad variety of parameter combinations, identified the parameter combinations giving acceptable agreement for each experiment, for the exponential and the linear burning profiles.

The investigated experiments were: ENACCEF Run 153, THAI HD-22, HD-24, RUT HYV01, BMC Hx23, and HDR E12.3.2. An exponential or a linear burning profile refers to the time evolution of the reactant concentration. As a result of this study, two sets of model input parameters (for the two burning profiles) with the best overall agreement with all six experiments and the uncertainty ranges for the input parameters were determined. These are given in the table below [6]:

Table 1

Default values and the uncertainty range for the FRONT model input parameters

Parameter	Description	Default value	Uncertainty range	Distribution	Correla-tion
DTRL	Integral scale of turbulence in vertical direction (Peters correlation)	0.001	[0.001;0.01]	Uniform on [0.001;0.003]; Triangle on [0.003;0.01], max. at 0.003	
TURLEN_H	Integral scale of turbulence in horizontal direction	0.001	[0.001;0.01]		
TURW	Turbulence decay coefficient	0.95	[0.9;1]	Triangle, max 1; or Uniform	

Uncertainty range for the exponential burning profile (model option COMO=EXPO)

REYEXP	n in the correlation for turbulence generation	-0.13	[-0.25;-0.01]	Uniform	Pearson coefficient r_{XY}= 0.75
REYFAC	C in correlation for u`	1.1	[0.1;2.5]	Uniform	

Uncertainty range for the linear burning profile (model option COMO=LINEAR)

REYEXP	n in correlation for u`	-0.13	[-0.2;-0.01]	Uniform	r_{XY}=0.65
REYFAC	C in correlation for u`	2.5	[0.1;4]	Uniform	

The THAI test facility [4] and the corresponding nodalization used in ASTEC are shown in Fig. 1. The (empty) test vessel is represented by 24 control volumes with 13 axial levels to include the thermocouples location. For test HD-23 with downward burn direction, the flame front propagation determined by the flame arrival at the locations of the fast thermocouples is illustrated in Fig. 1 (right upper part) [4].

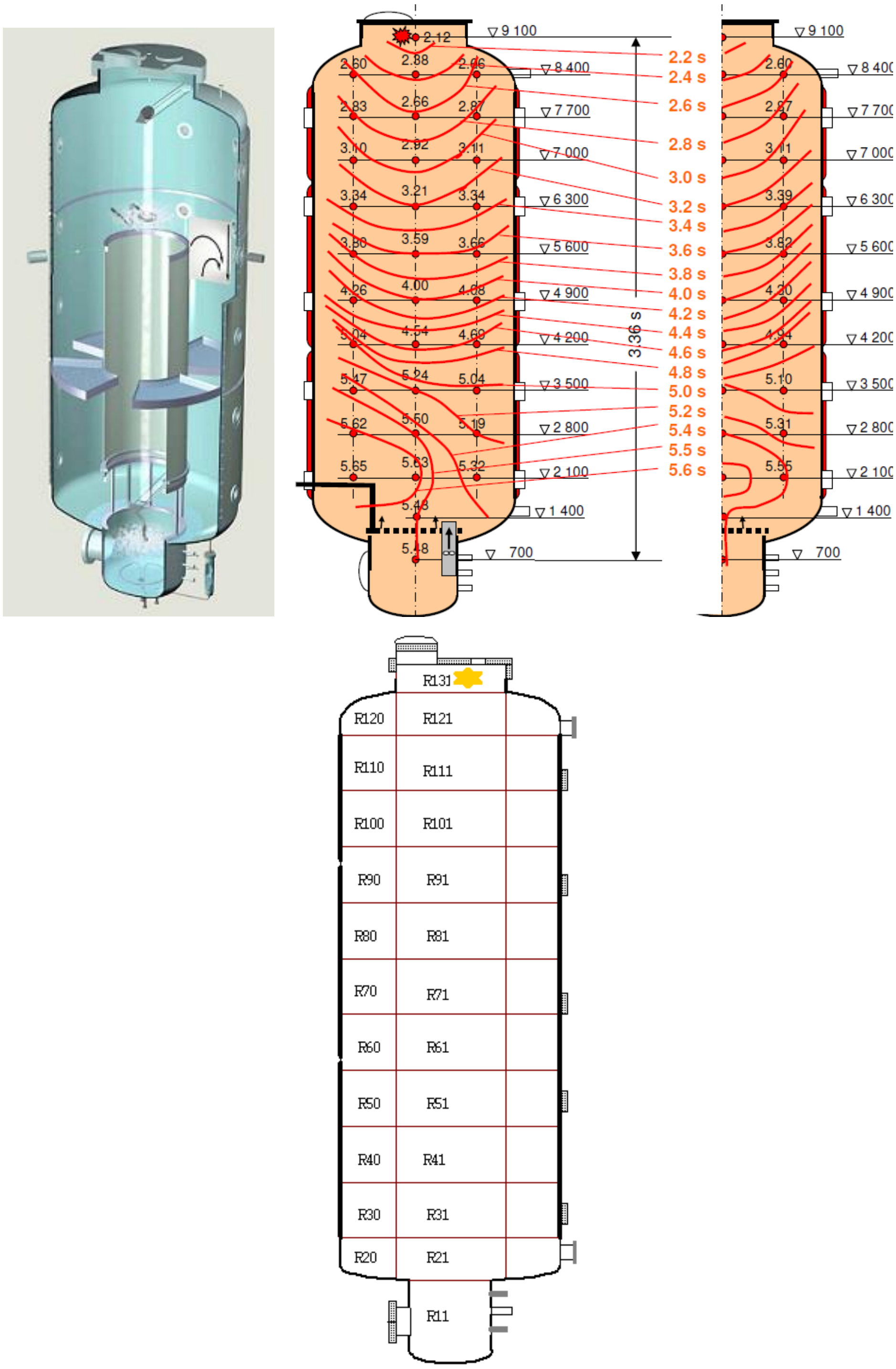

Fig. 1. THAI test facility [4] (left upper view), HD-23 flame front propagation along the vessel as isochrones [4] (right upper view), and nodalization used for ASTEC calculations (center lower view)

4.1 Calculation results with the exponential combustion profile option

The results of the calculation of the HD-22 test with the default set of model parameters listed in Table 1, assuming an exponential burning profile, are presented in Fig. 2. An exponential combustion profile is the typical evolution in time for a chemical reaction in laboratory experiments.

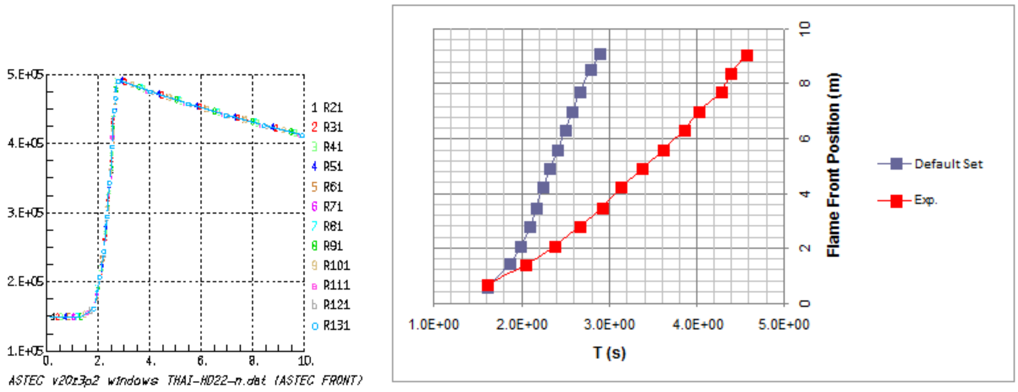

Fig. 2 THAI HD-22: Pressure (left side) and flame position on vessel axis (right side) calculated with the default set of parameters (COMO=EXPO)

The left side of the figure shows the calculated pressure evolution. The right side of this figure shows the flame front position along the vessel central axis as a function of time, the experimental measurements (red) and the ASTEC calculation results (dark blue).

The deflagration velocity and the gradient of the pressure increase for this test are overestimated with the default set of values for the model parameters. This is because the default values for REYEXP and REYFAC are greater than the respective range of parameter pairs suitable for the THAI HD-22 experiment determined in [6]. The peak pressure is reproduced with this set of parameter values. Due to the Lumped Parameter modeling, the acoustic pressure oscillations observed in the experiment cannot be reproduced in the calculation. The experimental results related to the pressure transient are found in [4]. In the present paper, the values for the Liu-McFarlane correlation were taken from the zone with the initial temperature of the accordant zone, but with the larger hydrogen concentration.

The calculated pressure profile and the average flame speed (Fig. 3) with REYEXP set to -0.119, REYFAC set to 0.168 and with the value of TURW equal to 0.9 show a good coincidence with the experimental data.

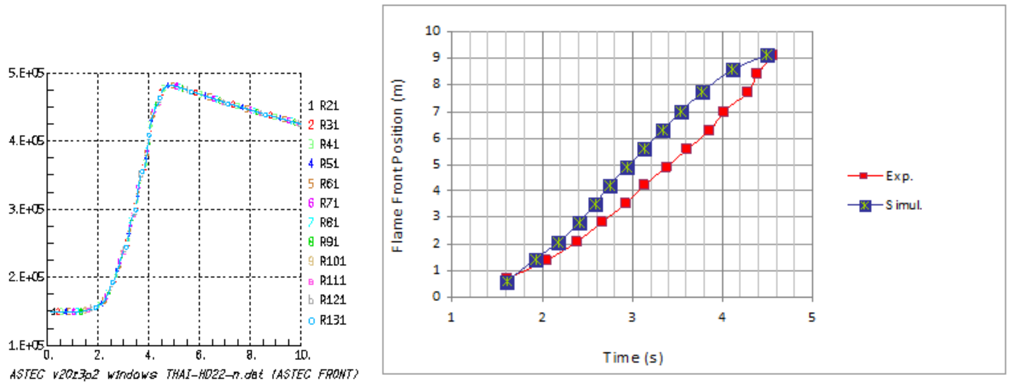

Fig. 3 THAI HD-22: Pressure (left side) and flame position on vessel axis (right side)

The calculation results for the HD-23 test with the set of default values for the model parameters, assuming an exponential burning profile in time, are presented in Fig. 4 and Fig. 5. The left side of Fig. 4 shows the calculated pressure evolution during the deflagration. The right side of this figure gives a comparison between the experimental measurements (red) and the ASTEC calculation (blue) for the time evolution of the flame front position in the centerline of the vessel. Fig. 5 (left) shows the calculated temperatures versus time in the middle of the vessel and near the vessel wall at the elevation 2.1 m and 4.9 m. The right side of this figure gives the temperature transient in the middle of vessel at 8.4 m. The pressure and temperature transients observed in the experiment HD-23 are found in [4]. The calculation with the default parameter values slightly underestimates the deflagration velocity and the gradient of the pressure increase. But nevertheless, the agreement between the calculation and the experiment is rather good. Simulated average flame velocity when the flame propagation downward along the central axis of the vessel reaches the elevation of 2.8 m is around -1.7 m/s. The temperature peak is overestimated.

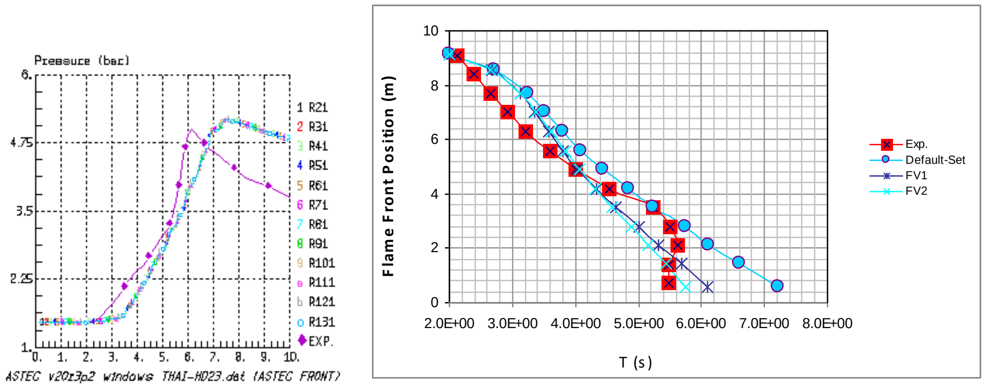

Fig. 4 THAI HD-23: Pressure transient (left side) and flame position on vessel axis (right side) calculated and observed in experiment

There are numerous combinations of REYEXP and REYFAC giving more or less acceptable agreement with the experimental data. For HD-23, Fig. 4, right side, shows the calculation results for two other calculations using the parameter DTRL/TURLEN_H (integral scale of turbulence) set to 0.001 and the parameter TURW (turbulence transfer from junction to adjacent junction) set to 0.95.

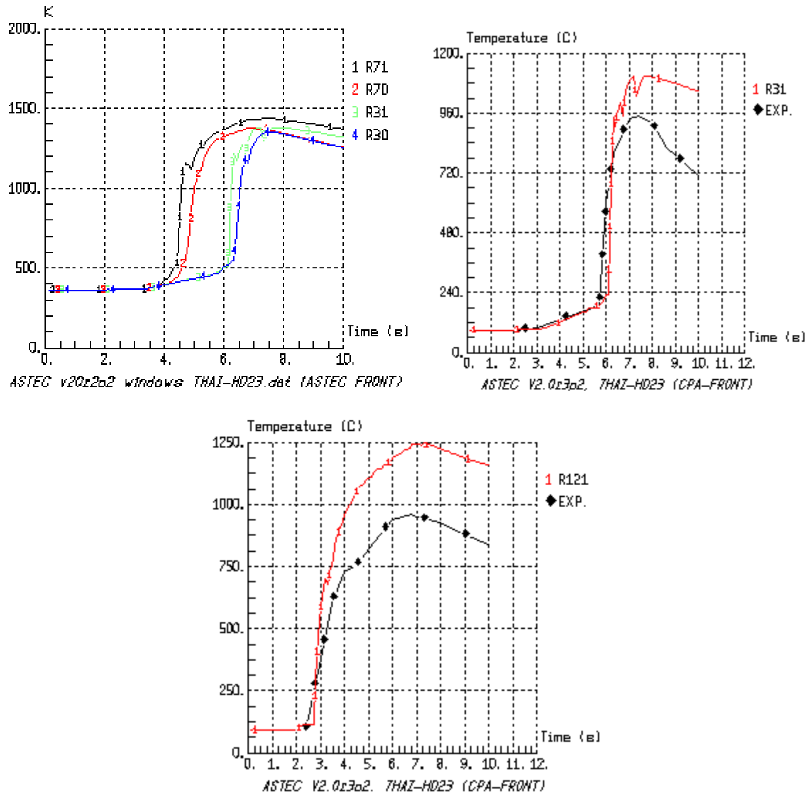

Fig. 5 THAI HD-23: Temperatures in the middle of the vessel and near the wall at elevation 2.1 m and 4.9 m (left and center) and in the middle of the vessel at 8.4 m (right)

The light blue line in this figure corresponds to the calculation using REYEXP set to -0.1 and REYFAC set to 1.1, while the violet line corresponds to the calculation with the value of the parameter REYEXP equal to -0.175 and the value of REYFAC equal to 2.5. For both calculations, the average flame velocity in the midldle of the vessel is in good agreement with the measured data

Fig. 6 gives the ranges of acceptable pairs REYEXP-REYFAC for suitable simulation of the THAI HD-23 test when considering the agreement with the measured pressure peak as well as when considering the agreement with the measured flame front position.

The dotted lines in this diagram give the upper boundaries of the ranges, while the straight lines represent the lower boundaries. The area between the dark blue lines (including both lines) indicates the range of pairs of REYFAC and |REYEXP|, which give more or less acceptable agreement between calculated and measured pressure peak for a value for DTRL set to 1 mm. For the same value of DTRL, the light blue lines represent the boundaries of the range of parameter pairs giving more or less acceptable agreement with the measured flame velocity. The brown lines indicate the range of parameter pairs giving acceptable agreement with the measured flame velocity for DTRL set to 3 mm. The violet point in the diagram stands for the default parameter pair REYEXP-REYFAC. The calculations were performed with the parameter TURW set to 0.95.

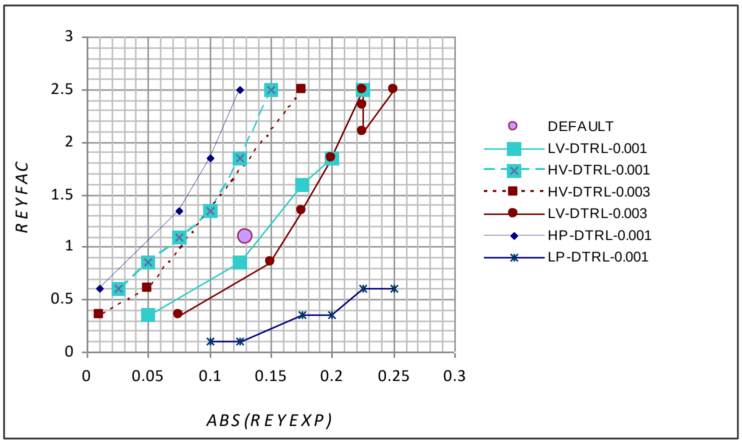

Fig. 6 THAI HD-23: Pairs of input parameters REYEXP-REYFAC with acceptable agreement with the measured pressure peak (dark blue) and flame front position (light blue and brown)

There are some differences between the calculated range of parameter pairs for which the flame velocity is in acceptable agreement with the experiment HD-23 (Fig. 6) and the range for the experiment HD-22 from the reference [6]. These differences are probably due to the data used from available literature.

4.2 Calculation results with the linear combustion profile option

Fig. 7 gives, for the test HD-22, the results of the calculations performed with the default parameter values listed in Table 1, assuming a linear burning profile in time in the control volumes. These include the pressure transient and the vertical flame front propagation along the vessel axis. In this case, the calculation slightly underestimates the deflagration velocity and the gradient of the pressure increase.

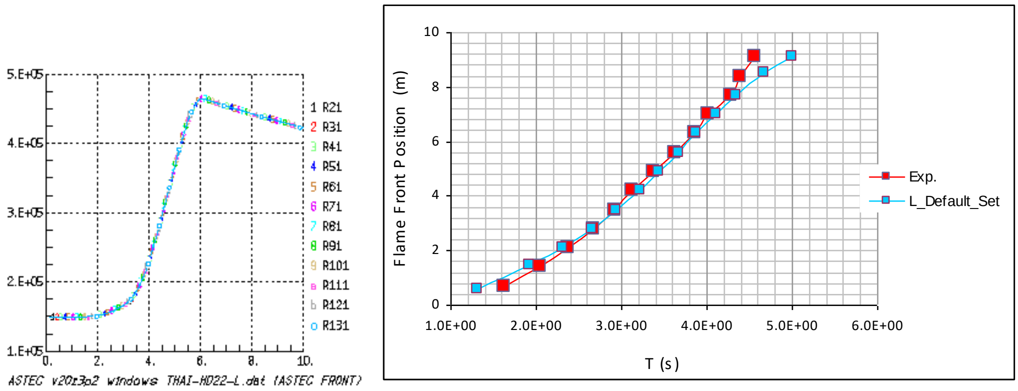

Fig. 7 THAI HD-22: Pressure transient (left) and flame propagation in the center of vessel (right) calculated with the default set (COMO=LINEAR) and experimental measurements

In the case of the test HD-23, the calculation results with the default values for the model input parameters assuming a linear combustion profile in time are presented in Fig. 8 and Fig. 9. These figures show the transients of flame front motion, pressure and temperature in the middle of the vessel at the elevation of 2.1 m and 8.4 m.

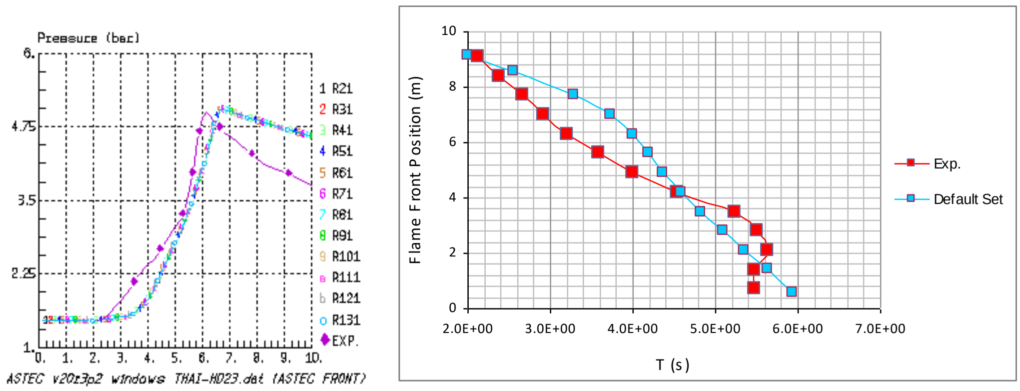

Fig. 8 THAI HD-23: Pressure transient (left) and flame position on vessel axis (right) calculated with the default parameter set (COMO=LINEAR) and experimental measurements

The calculation again slightly underestimates the deflagration velocity and the gradient of the pressure increase. However, the agreement between the ASTEC calculation and the experiment is good. The peak temperature is overestimated with the default values for a linear burning profile.

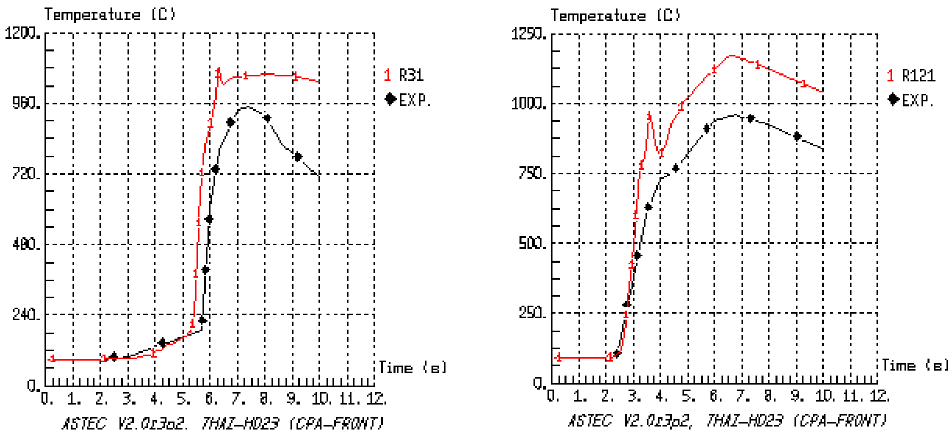

Fig. 9 THAI HD-23: Temperature transients in the middle of the vessel at elevation 2.1 m (left side) and at 8.4 m (right side)

Fig. 10 gives the ranges of acceptable pairs REYEXP-REYFAC resulting from the measured flame front position and the pressure for the HD-23 experiment assuming a linear burning profile in time. The calculations were performed with the parameter DTRL set to 1mm and with TURW set to 0.95.

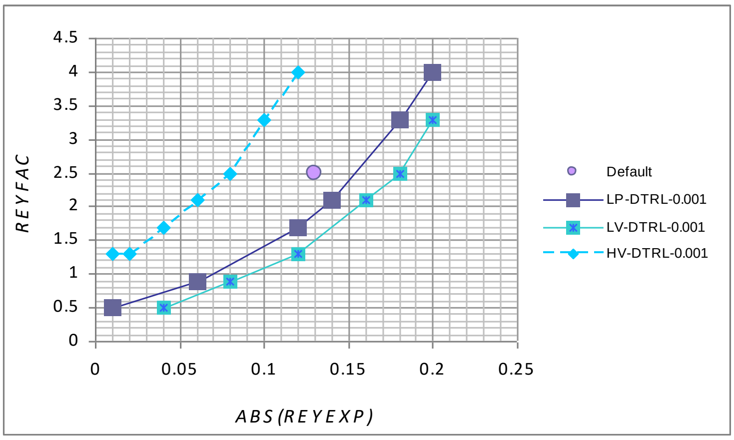

Fig. 10 THAI HD-23: Pairs of input parameters REYEXP-REYFAC with acceptable agreement with the measured pressure peak (dark blue) and flame front position (light blue)

The dark blue line connects the pairs of REYFAC and |REYEXP|, which give just “low enough” pressure peak. The area between the light blue lines indicates the range of parameter pairs, which give more or less acceptable agreement between calculated and measured flame velocity. The boundary lines of both sides represent values which are not suitable.

4. Conclusions

This paper presents the results of the calculations of the slow deflagration tests HD-22 and HD-23 with the FRONT model of the CPA module of the ASTECv2.0 code in comparison with the experimental data. The calculations were performed assuming an exponential burning profile in time in the control volumes as well as a linear burning profile.

From the comparison of measured and calculated data, the following conclusion can be drawn. For test HD-23, the simulated results of FRONT model with the default values for the input (empirical) parameters, assuming an exponential burning profile in time, are in acceptable agreement with test data. For this test, the simulations with the default parameter values slightly underestimate the flame front velocity and the gradient of the pressure increase. From comparison of the experimental measurements for pressure peak and flame front position with the calculation results, the parameter combinations giving acceptable agreement were identified for this test. For test HD-22, the deflagration velocity along the vessel axis and the gradient of the pressure increase are overestimated with this set of values for model parameters. The peak pressure is well reproduced in both cases. Test simulations showing a good agreement with the experimental data are also presented. The overall agreement between the default parameter calculations and the measurements is better for the case when a linear combustion profile in time is assumed in each control volume than for the case of an exponential profile. The gas temperatures are overestimated in all calculations.

R E F E R E N C E S

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