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SIMULATION OF THAI HD-12 AND HD-22 WITH THE FLAME FRONT MODEL OF ASTEC USING DIFFERENT CORRELATIONS FOR THE TURBULENT BURNING VELOCITY

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Abstract

In this paper the simulation of the tests THAI HD-12 and HD-22 with the flame front model (FRONT) of ASTEC using different approaches for the turbulent burning velocity is treated. Results of the simulations depend on the estimation of the turbulence intensity. Applying only one parameter set, the correlations indicate different behaviours. To show the influence of the turbulence intensity parameter, these were varied and thus, a good agreement to the experiment can be achieved with each correlation. In addition, a recommendation for the models parameter will be given for the actual used correlation according to Peters.

KEYWORDS: Combustion, Turbulence, THAI, ASTEC, Nuclear Safety

Introduction

Effects of possible hydrogen combustion could be important for late phases of hypothetical loss-of-coolant accidents, leading to an overheated core and thereby to a reaction between steam and the cladding material of the fuel rods. Due to this zircon steam oxidation, hydrogen is produced in the core, which can be released from the primary cooling circuit, through a leak into the containment. In case of an ignition of a flammable mixture, pressure as well as temperature increases and the overall convection in the containment is enlarged (relevant for the source term). The course of combustion depends amongst other on the hydrogen and steam content as well as on their distribution in the containment atmosphere. Moreover, the burning rate is increased by turbulence, occurring in the path of the flame front. Due to the higher burning rate, the energy of the fuel is released in a shorter time, causing a steeper pressure and temperature gradient and thus, the load on containment structures is increased. There are several measures to mitigate the formation of mixtures containing high hydrogen concentrations, e.g. the containment inertisation in boiling water reactors and passive autocatalytic recombiners in pressurised water reactors, but combustion cannot be ruled out completely in range of low hydrogen concentrations [1].

Phenomena of flame acceleration were investigated within the "International Standard Problem of Hydrogen Combustion (ISP-49)" by participants of 14 organisations from 7 countries. In order to evaluate and analyse models for hydrogen deflagration in CFD as well as lumped parameter codes experiments in the THAI and the ENACCEF facility were used for blind and post test simulations. This article treats the simulation of the test THAI HD-12 and THAI HD-22 with the flame front model of the integral lumped parameter code ASTEC. Amongst other this model was used in the ISP-49 by participants of the Gesellschaft für Anlagen- and Reaktorsicherheit mbH (GRS) and the Ruhr-Universität Bochum. Results of the simulations were in good agreement to the experimental data, but different parameters for the modeling of turbulence in the simulation of both tests have to be used (see chapter 2.2). These observations were made in simulations of further tests, within a combustion benchmark in the NoE SARNET 2, too. It was observed, that in the simulation of deflagration tests considering high turbulence a stronger change of these parameters is necessary. Up to now, the model was developed by GRS only. As a first step in the modeling of RUB, the influence of different correlations for the turbulent burning velocity on the simulation results will be investigated in this paper. Like in a number of combustion models, the turbulent burning velocity is one of the main parameters in the FRONT model. In addition to the used one, four additional correlations for the turbulent burning velocity were implemented in the model. The THAI HD-12 and HD-22 tests were chosen for first simulations, because they are characterised by slow combustion. In the following, the THAI test facility as well as the tests HD-12 and HD-22 is described. Afterwards the simulation results including the model and different correlations for the turbulent burning velocity are analysed.

1. Experiments THAI HD-12 and THAI HD-22

The THAI HD-test series consist of 29 experiments, emphasizing investigations related to the phenomena of flame propagation up- and downwards directed, under different initial conditions like temperature, pressure, hydrogen and steam concentration [1]. These tests were performed in the THAI containment within the OECD-NEA THAI Project in order to gain further insight into phenomena of flame propagation and to provide necessary data for code validation. The THAI containment operated by Becker Technologies GmbH (Eschborn, Germany) has a volume of about 60 m^3, a height of 9.2 m and consists of mainly three parts; the bottom, the middle cylinder and the top (see Figure 1). Main part of the facility is the middle cylinder, which has a diameter of 3.156 m and a height of about 6.8 m [1]. Vessel bottom and top, which have a smaller diameter and a lower height than the middle part, are mounted by dished heads. All walls of the facility were made of stainless steel and completely enveloped by a rock wool layer. At the middle part of the facility, a heating/cooling system was installed, working with thermal oil flowing through a gap between additional structures. Figure 1 illustrates a sketch of the THAI facility on the left side and on the right side the model used for all simulations in ASTEC (described in chapter 2.3). The sketch shows the THAI facility in basic configuration, including an inner cylinder and condensate trays, which were removed for the THAI HD-test series. Additional components for this test series were a fan and spark igniters, which are located in the vessel bottom and the vessel top. The fan was switched on, to homogenise the flammable mixture in case of a uniform distribution of the hydrogen and/or steam inside the facility. During the test, different devices were used to measure temperature, pressure and the flame front propagation. The hydrogen concentration was measured before ignition and after the test.

The tests HD-12 and HD-22 were performed at an elevated pressure of about 1.5 bar and the mixture was ignited at the vessel bottom. In the test HD-12 the initial temperature was about 20°C and the mixture composed of 8 vol.-% hydrogen in dry air. In contrast to HD-12, the temperature of the mixture in the test HD-22, consisting of about 10 vol.-% hydrogen and 25 vol.-% steam, was about 90°C. The differences between both tests are the initial temperature, the hydrogen as well as the steam concentration – while the atmosphere in the test HD-12 is nearly dry, it is half-saturated in the test HD-22. In both tests upward flame propagation in a mixture close to the ignition limit is investigated. Figure 2 shows the hypothetical flame propagation by isochrones, reconstructed from signals of fast thermocouples at different elevations in the vessel. The arrival of the flame front at a specified location was detected by the first sharp temperature increase at one sensor [1, 2].

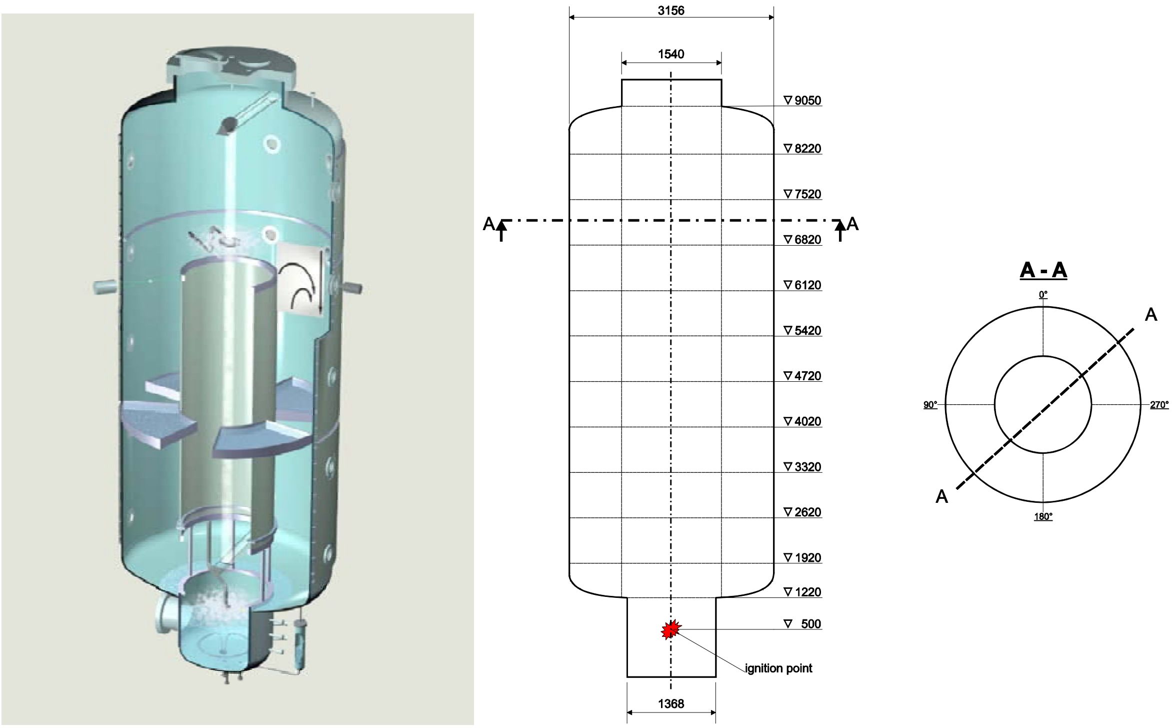

Figure 1 Sketch of THAI facility [1] and model of the THAI facility in ASTEC

From the first sensor above ignition point at 0.7 m to the last one, in the top of the facility at a height of 9.1 m, it took about 4.04 s in HD-12 and about 2.94 s in HD-22. Thus, the flame velocity is higher in HD-22 than in HD-12. In both tests, the flame was propagating firstly along the centre line of the vessel and then it expands to the sensors located at the sides. The time lag for reaching the sensors at the sides, when the flame has already passed the middle ones, decreases with growing elevation in the vessel. This behaviour lasts significantly up to an elevation of 4.9 m in both tests. Afterwards, the flame spreads in horizontal as well as in vertical direction. In HD-22 the sensors in the upper as well as top part of the vessel are showing a temperature increase earlier than in HD-12. One significant observation can be made by considering two sensors on an elevation of 2.1 m, which are recording a later signal than the one, located in the area of the bottom at 9.1 m. Comparing the flame propagation, which appears unsymmetrical in both cases, the flame propagation is more erratic in HD-12. The effect of the earlier flame arrival and thereby the later signal of the sensors at the side in the lower part of the vessel can be explained by the effect of buoyancy. Due to this influence, the flame is accelerated in vertical direction to the top, leading to an increase of turbulence in the surrounding unburned gas, which causes propagation in upward as well as in downward direction [1].

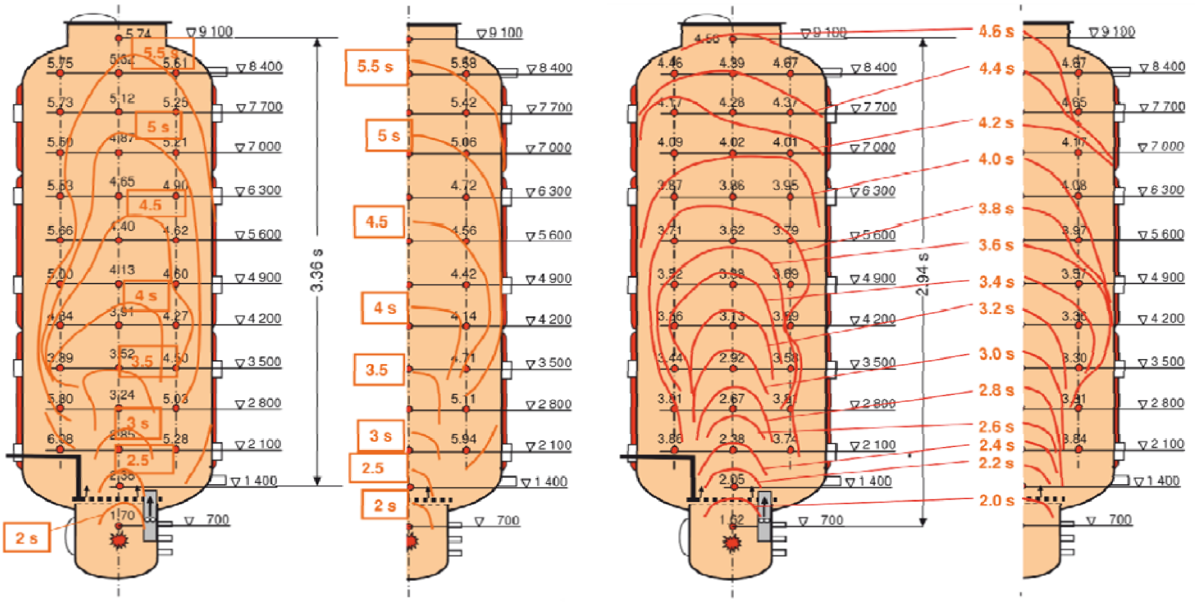

Figure 2 Flame propagation by isochrones of the test THAI HD-12 (left) [2] and THAI HD-22 (right) [1]

To introduce both experiments, the theoretical flame propagation was discussed in this chapter. Further experimental results, as the pressure and the flame arrival at the vessel axis, are used for evaluation of the simulation results.

2. Simulation of the experiments THAI HD-12 and HD-22

For the simulation of both experiments, the flame front model (also called FRONT) of the integral lumped parameter code ASTEC was used. ASTEC means Accident Source Term Evaluation Code and is a joint development of the French Institut de Radioprotection et de Sûreté Nucléaire (IRSN) and the GRS. With ASTEC an entire severe accident sequence in nuclear power plants can be simulated, using different modules for phenomena in the "in-vessel" as well as the "ex-vessel" part. One main characteristic of a lumped parameter code is that changes of physical quantities in one zone are assumed to be time dependent only. During simulations equations for heat and mass transfer are solved and the result in each defined volume (zones) is referred to the centre (node). To enable heat and mass transfer between zones, junctions have to be set between them. Further inputs (structures) have to be defined to account heat transfer between walls and the fluid in zones e.g. the thermal conductivity of the material.
In comparison to CFD and other computer codes, the used volumes in lumped parameter codes are larger and consequently small scale phenomena like viscous boundary layers in turbulent flows cannot be resolved. On the one hand, the coarser resolution of the geometry in the lumped parameter model leads to a less detailed solution of the simulation, but on the other hand, it en-

ables a shorter calculation time. Hence these computer codes are suitable for plant applications and parametric studies.

2.1 Description of the FRONT model

FRONT is the latest one of five hydrogen deflagration models implemented in ASTEC and released with version 2.0 at mid of 2009 [3]. The combustion models differ in the number and complexity of the user input parameters and the detail, in which they describe the process. In principle the FRONT model is an add-on to the older COMB model. COMB calculates the effects of combustion by solving equations for heat- and mass balance in zones, without considering flame propagation between them. Using COMB in standalone, the user has to define the beginning and the duration of the combustion process [3]. If the FRONT model is activated in the input data set of ASTEC, it estimates the start of combustion and the burning duration for every defined zone by simulating one-dimensional flame propagation through junctions. According to this model feature, zones have to be connected by junctions and the combustion propagates sequentially from the first one, in which the user defines the ignition, to adjacent ones. The theoretical flame starts always from beginning to the end of a junction, which is defined by the next node. Once the flame reaches the end of a junction, the burning duration and the time is transferred to COMB. The burning duration respectively the burning rate as well as the flame speed is determined with the turbulent burning velocity and hence the turbulent burning model is one of the important parameters of the model. Actually, the model uses the turbulent burning velocity according to Peters which takes turbulence into account with the turbulence intensity u' and the integral scale of turbulence l (see Equation 2 and Equation 3) [3, 4].
ASTEC does not consider momentum balance [5], but this is necessary for estimation of the integral scale of turbulence l and the turbulence intensity u'. Therefore, the integral scale of turbulence is calculated with the cross section area of junctions and the turbulence intensity u' is estimated by a simplified algebraic equation [3]:

$$u' = C \cdot U_m \cdot (Re)^n \qquad (1)$$

with	u'	[m/s]	Turbulence intensity,
	C	[-]	Dimensionless Coefficient,
	U_m	[m/s]	Average gas velocity,
	Re	[-]	Reynolds number of average gas velocity,
	n	[-]	Dimensionless Coefficient.

The turbulence intensity u' (see Eq.1) is calculated by a coefficient C, an exponent n, the averaged gas velocity U_m and the Reynolds number Re of the gas flow in a junction. The user has the ability to change values of the exponent n and the factor C in the input data set [3]. The delivered version of ASTEC V2.0r1 contains one parameter data set (C = 1.7 and n = -0.12) in the test case of the FRONT model. In some cases this parameters had been changed in former investigations to achieve better agreement to the experimental data.

2.2 Implemented correlations for the turbulent burning velocity

Like in the FRONT model, the turbulent burning velocity is one of the main parameters in a number of combustion models. In CFD codes the so-called Flame Speed Closure models (FSC) uses the turbulent burning velocity to close set of equations which arises from the consideration of reaction progress variables in addition to turbulence [6]. The following equations for the turbulent burning velocity were used instead of the Peters equation in the FRONT model for the simulation of the THAI HD-12 and HD-22 experiments:

Peters [3, 4]: $$\frac{S_T}{S_L} = (1+\sigma) \quad (2)$$

with $$\sigma^2 + 0.39 \cdot \sigma - 0.78 \cdot \frac{u' \cdot l_f}{S_L \cdot l} \quad (3)$$

Kawanabe [6,7]: $$\frac{S_T}{S_L} = 1 + 1.25 \cdot \left(\frac{u'}{S_L}\right)^{0.7} \quad (4)$$

Schmid [6,7,8]: $$\frac{S_T}{S_L} = 1 + \frac{u'}{S_L} \cdot (1 + Da^{-2})^{-0.25} \quad (5)$$

Bradley modified [7]: $$\frac{S_T}{S_L} = u'^{0.75} \cdot (l \cdot \frac{{S_L}^2}{\chi})^{0.25} \quad (6)$$

Zimont [6,9]: $$\frac{S_T}{S_L} = A \cdot u' \cdot Da^{0.25} \qquad A = 0.6 \quad (7)$$

with	S_T	[m/s]	Turbulent burning velocity,
	S_L	[m/s]	Laminar burning velocity,
	σ	[-]	Surface area ratio,
	l	[m]	Integral scale of turbulence,
	l_f	[m]	Laminar flame thickness,
	A	[-]	Coefficient in the Zimont Correlation,
	χ	[m²/s]	Thermal diffusivity.
	Da	[-]	Damköhler number, Da = $(u' \cdot l)/(S_L \cdot l_f)$ [4]

Except equation 2, all the turbulent burning velocity equations are expressed with the integral scale of turbulence l, which is also included in the definition of the Damköhler number. The Damköhler number is defined by the relation between the chemical time scale and the turbulent time scale [8]. Furthermore, the equations contain the laminar burning velocity S_L, the laminar flame thickness l_f. Equation 2 gives the turbulent burning velocity with the mean flame brush thickness σ, which is calculated by solving Equation 3. The value of the dimensionless parameter A in the equation according to Zimont was taken from reference [9] for hydrogen air mixtures. More information to the considered equations can be found in [3, 4, 6, 7, 8].

2.3 Modeling of the considered experiments in the THAI facility

As it can be seen Figure 1 (right), the nodalisation of the THAI facility, used for the simulation of the tests THAI HD-12 and HD-22 consists of 57 zones. One zone is in the bottom and another in the top of the facility and the remaining 55 are located in the middle part of the facility, which is divided into 11 axial layers. The locations of the zone centers are the same as the measurement devices. The layers are further subdivided into 5 zones, whereas one cylindrical shaped zone is in the middle, which has the diameter of the vessel top and lies at the centre axis of the vessel. The cylindrical shaped zones are surrounded by 4 ring zones with an angle of 90° forming together a ring. Junctions are defined with the cross section area of the adjacent inter faces, a flow resistance coefficient of 1.0 and a length according to the vertical or horizontal distance of the centre, respectively. The walls of the THAI vessel are modeled as specified in the description [1, 2] – for the thermal oil additional structures are used.
Within ISP-49 two nodalisations had been used by RUB, from which only one is taken for the evaluation of the turbulent burning velocities discussed in chapter 2.2. The influence on the simulation results of two considered nodalisations were discussed in [10]. The nodalisations vary in the number of zones within the ring. Main differences of the simulation results are the flame velocity and the pressure progression, which depends on the overall burning rate. The flame speed was a little higher and the pressure gradient increased sharper in the simulations with two ring zones – but in summary, the results did not show strong deviations compared to each other.

2.4 Results using one parameter set for the turbulence intensity

In a first evaluation step of the correlations of the turbulent burning velocity implemented in FRONT, simulations were performed with one parameter set of the coefficient C and the exponent n of Equation 1. In these simulations C is set to 1.7 and n has a value of -0.12, according to the delivered test case of ASTEC V2.0r1. To compare the simulation results to the measurements, a time shift of the simulation data was made, because the ignition time in the experiment is not know. Due to this shift, the time for arrival of the flame front at the second sensor above ignition point (1.4 m) is in all simulations the same and fits to the experimental data. Owing to the fact that the FRONT model does not simulate a multidimensional flame, the time for the arrival at zone centers is plotted by the ignition time for each zone and taken for comparison for the flame arrival in the simulations. Figure 3 and Figure 4 depict the results of the flame propagation at the center line of THAI HD-12 and HD-22. Compared to the experiments, the simulations with different turbulent burning velocities show a quite different behavior and thereby they can be categorized into three groups - fast, intermediary and slow flame progression related to the measured values. Using the correlation of Bradley and Zimont, the arrival of the flame front at different elevations in the simulations appears the earliest and thereby they are significantly overpredicted in both experiments. Kawanabe and Schmid are in very good agreement to the shape of the measured curve, but in both cases the time of the arrival at the last sensor are underestimated by about 0.5 s in HD-12 and about 1 s for HD-22. Furthermore, the flame speed in the test HD-22 correlates less to the measured one than in HD-12. The flame arrival of the actually implemented Peters correlation is in between the results discussed before and has a too steep curve gradient in case of HD-12 and a sufficient course in comparison to HD-22, whereas in the last mentioned test the arrival at the last sensor is predicted very well.

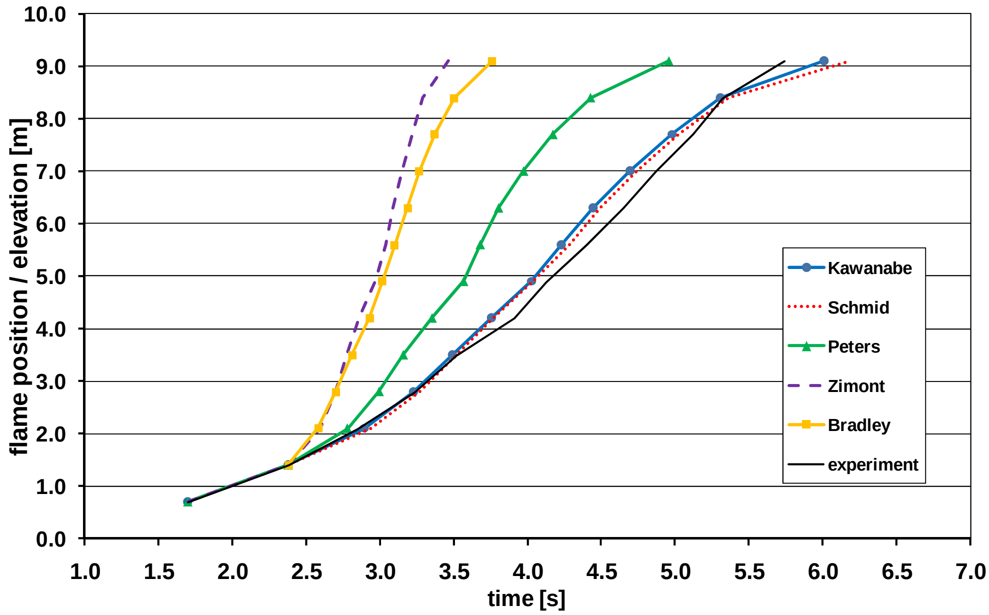

Figure 3 Simulated and measured flame propagation along the center THAI HD-12

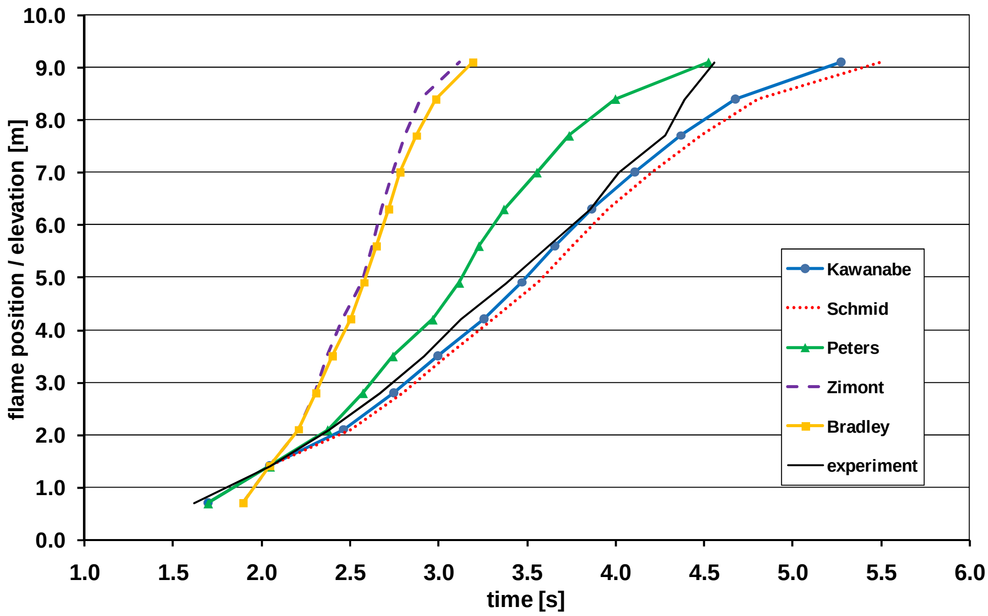

Figure 4 Simulated and measured flame propagation along the center THAI HD-22

Figure 5 and Figure 6 illustrate the pressure progression of HD-12 and HD-22. In HD-12 the pressure rises at first very slight and then with a seemingly linear gradient until it reaches the maximum of about 4.9 bar. The pressure in the test HD-22 rises sharper, more erratic and more unsteady related to HD-12; firstly with a sharp gradient and then it decreases until reaching the maximum of about 4.7 bar. After reaching the maximum, the pressure is reduced. This can be ascribed to heat removal from the vessel walls to the ambient.

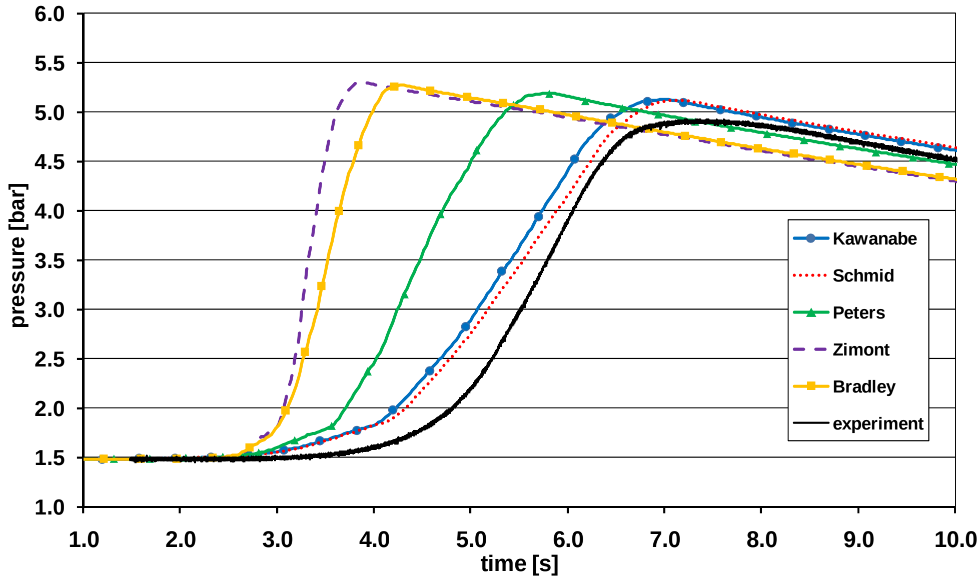

Figure 5 Simulated and measured pressure in THAI HD-12

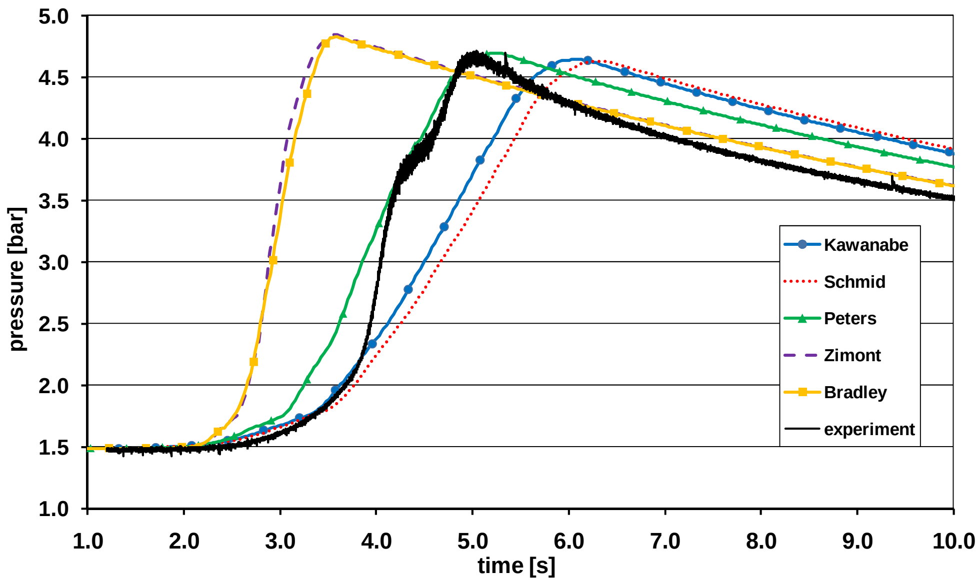

Figure 6 Simulated and measured pressure in THAI HD-22

The behavior of the flame front arrival using the different correlations is reflected in the course of the pressure in both tests. The experimental pressure progression is overpredicted in case of the simulations with the correlations of Bradley and Zimont. Using the correlations of Kawanabe and Schmid, the pressure is well reproduced for HD-12 and underestimated in HD-22. With the correlation of Peters, the FRONT model calculates a too early pressure increase, whereas results are qualitatively good in the test HD-12 and the last phase of HD-22. In the early phase of the pressure progression of HD-22 the gradient of the pressure is underestimated, but the flame reaches the last sensor in range of the experimental arrival, the time for the maximum pressure is nearly the same in the simulation. Moreover the values of the maximum pressure and the following pressure reduction are well reproduced in all simulations and for both tests.

2.5 Results with adapted parameter set for the turbulence intensity

In order to show the influence of the turbulence intensity and to check the applicability of the chosen correlations for the turbulent burning velocity, the parameters of Equation 1 were varied. Thereby one data set for Zimont and Bradley (C = 0.3; n = -0.05), one for Kawanabe and Schmid (C = 1.5; n = -0.07) and another for Peters (C = 1.5; n = -0.15) were defined. Due to the limitation of this paper, the results of the simulations with adapted parameters for turbulence intensity, depicted in Figure 7 and Figure 8, are treated for the HD-22 experiment only. By adapting the parameter of the turbulence intensity, the flame propagation is reproduced well with all correlations. Except the simulations using the modified Bradley correlation all are close to the experimental curve, whereas the best agreement results in the simulation based on the Peters correlation. While the simulation with Bradley's correlation overestimates the flame arrival time up to an elevation of 2.1 m, the other ones deviate significantly up to an elevation of 8.1 m and reach the last elevation later compared to the experiment.

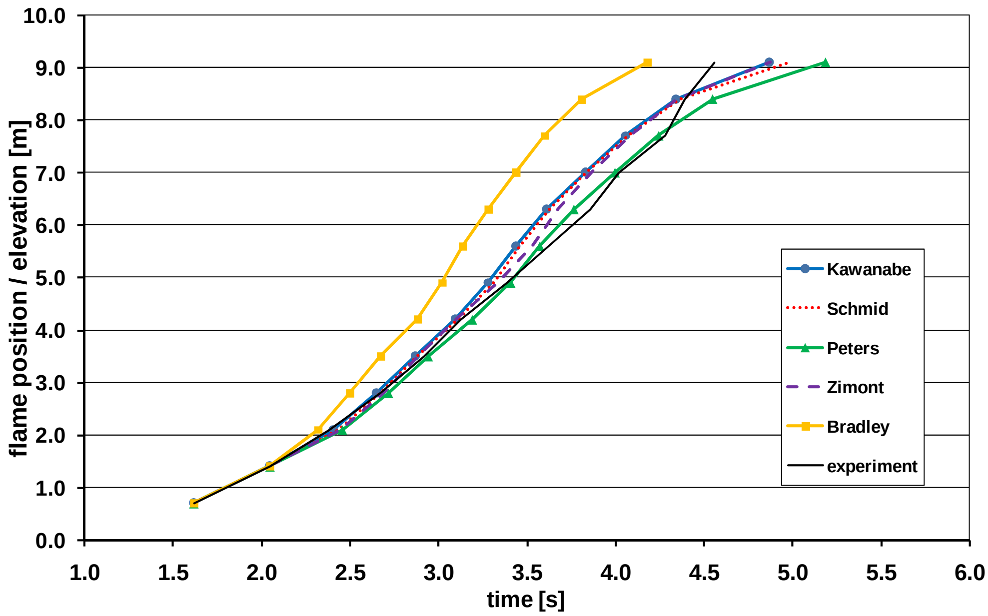

Figure 7 Simulated and measured flame propagation along the center THAI HD-22

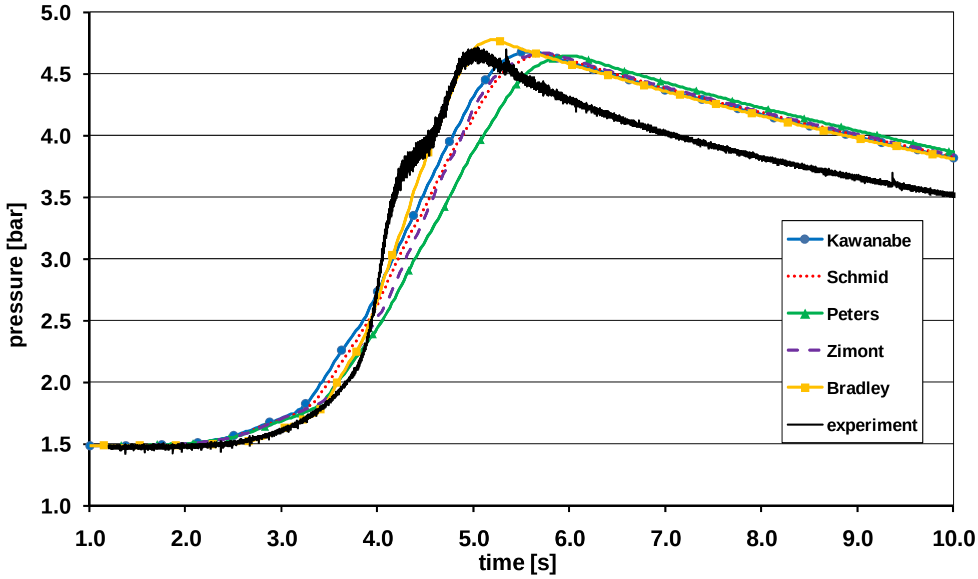

Figure 8 Simulated and measured pressure in THAI HD-22

Like before same trends between the flame arrival and the pressure progression can be recognized. According to the good result in the flame propagation, the pressure is in good agreement to the experiment too. The best estimation of the pressure progression, regarding the gradient and the time for the maximum is achieved with the correlation according to Bradley.

3. Conclusions

The simulations of the test THAI HD-12 and HD-22 using five correlations for the turbulent burning velocity show that this is a sensitive parameter in the FRONT model. Using the same parameter data set to estimate the turbulence intensity, the results are quite different related to the progression of the pressure as well as the flame arrival at different elevations in the THAI vessel. Overall the results like pressure maximum and the following decrease are in good agreement to the experiment. In case of a well predicted flame arrival at different elevations of the vessel axis, like in the simulation with THAI HD-12 using the Schmid as well as the Kawanabe equation, the model calculates a less steep gradient of the pressure compared to the experiment. This behavior can be deduced from the time for the ignition of the side zones and thereby the global burning rate in the simulations. By applying another nodalisation of the THAI vessel with a smaller number of ring zones, the pressure gradient is slightly steeper and thereby the results may be improved.

Simulations performed in a second step show that, with an adaption of the turbulence intensity, the results can be refined for every correlation. The resulting pressure and the flame arrival at different elevations at the center line of the THAI vessel are reproduced well for all approaches except the correlation according to Bradley. The results got with the approach according to Bradley, can be improved by further adaption of these parameters. Due to this, the final evaluation of a correlation for the turbulent burning velocity used in the FRONT model has to be redone by using one approach for the turbulence intensity and considering experiments under different ini-

tial and geometrical conditions. As a first trend, the Schmid and the Kawanabe as well as the Peters correlation provide good results.
By using the delivered ASTEC Version 2.0r1 which uses the Peters correlation, the standard parameter set for the turbulence deliver good results which can be refined by another set (C=1.5 and n = -0.15), and therefore these are recommended firstly.

4. Acknowledgements

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