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Abstract

In a large number of validation calculations during the last decade it was shown that the COM3D code can satisfactorily predict all main characteristics of flame acceleration and flame propagation for mixtures in the range of concentrations from 11 to 30% vol. H_2 in air. For mixtures below 11% a demonstration of the conservatism of the calculated pressure loads would extend the applicability of the code to lean mixtures in the sense that at least bounding predictions can be made. The simulation of the experiment mc043, which was carried out in the course of the EU Fifth Framework Program Project HYCOM was used to demonstrate the main characteristics of the simulations with the COM3D code in the range of leaner mixtures. The paper describes the work which was performed with the aim to qualify the abilities of the COM3D code to provide reliable results for turbulent combustions in H_2-air mixtures with lower hydrogen concentrations. The paper includes: a description of the code combustion model; a description and experimental details of the experiment mc043; and a description of the simulation of the experiment mc043 and discussion of the obtained results.

Berechnung von Verbrennungsvorgängen in mageren H_2-Luft Gemischen: Konservativität der COM3D Ergebnisse

Zusammenfassung

In den letzten 10 Jahren wurde durch eine große Anzahl von Validierungsrechnungen gezeigt, dass der COM3D Code alle wesentlichen Merkmale der Flammenausbreitung und der Flammenbeschleunigung für Mischungen im Konzentrationsbereich von 11 bis 30% Vol. H_2 in Luft zufriedenstellend beschreiben kann. Eine Demonstration der Konservativität der berechneten Drucklasten bei Mischungen unterhalb 11% Vol. würde die Anwendbarkeit des Codes dahingehend erweitern, dass zumindest die maximalen Lasten abgeschätzt werden können. Die Berechnung des Experiments mc043, das innerhalb des Projektes HYCOM des 5. Rahmenprogramms der EU durchgeführt wurde, wurde benutzt, um die wesentlichen Merkmale der COM3D-Simulationen bei mageren Gemischen aufzuzeigen. Dieser Bericht beschreibt die Arbeiten, die mit dem Ziel durchgeführt wurden, den COM3D Code für turbulente Verbrennung in H_2-Luft-Gemischen bei niedrigen Wasserstoffkonzentrationen zu qualifizieren. Dieser Bericht beinhaltet: eine Beschreibung des Verbrennungsmodells, eine Beschreibung und experimentelle Details des Experiments mc043, eine Beschreibung der Simulation des Experiments mc043 und eine Diskussion der Ergebnisse.

The COM3D code was developed at FZK with the focus on the numerical simulation of reacting turbulent flows. The code solves the 3D unsteady, compressible Navier-Stokes equations using the standard (k, ε)-turbulence model and a modified eddy break-up (EBU) combustion model [1,2]. The numerical solver employs an explicit shock capturing second-order algorithm [3], realized on a rectangular equidistant mesh.

In a large number of validation calculations during the last decade it was shown that the COM3D code can satisfactorily predict all main characteristics of flame acceleration (FA) and flame propagation for mixtures in the range of concentrations from 11 to 30 % vol. H_2 in air [e.g. 4, 5]. For mixtures below 11 % a demonstration of the conservatism of the calculated pressure loads would extend the applicability of the code to lean mixtures in the sense that at least bounding predictions can be made. The simulation of the experiment mc043, which was carried out in the course of the EU Fifth Framework Program Project HYCOM was used to demonstrate the main characteristics of the simulations with the COM3D code in the range of leaner mixtures.

The current paper describes the work which was performed with the aim to qualify the abilities of the COM3D code to provide reliable (and/or conservative) results for turbulent combustions in H_2-air mixtures with lower hydrogen concentrations. The paper consists of the following sections:

- a description of the code combustion model;
- a description and experimental details of the experiment mc043;
- a description of the simulation of the experiment mc043 and discussion of the obtained results.

The results are summarized in the concluding section of the paper.

Combustion model in COM3D code

The modified EBU model extends the standard EBU model by taking into account the distinction between the movements of the flamelets and the turbulent flow. It has been shown [1] that the mean reaction rate strongly depends on the ratio of the turbulent kinetic energy k (measured in m^2/s^2) to the laminar flame velocity S_L (m/s) when $k^{1/2}$ is of the order of S_L, i.e. when the reaction rate is controlled not only by the mixing of turbulence (related to k), but also is influenced by the flamelet properties (related to S_L). Following [1], the modified formula for the mean reaction rate $\tilde{\omega}_j$ of component j with mass fraction Y_j (being initially equal to Y_j^0) reads

$$\tilde{\omega}_j = -\alpha \frac{C_{EBU}}{\tau_t} \tilde{Y}_j \left(1 - \frac{\tilde{Y}_j}{Y_j^0} \right) \qquad \text{with} \qquad \alpha = 1 + \frac{4.4}{1 + 3.2 \frac{k^{1/2}}{S_L}} \qquad \textbf{Eq. 1}$$

where τ_t is a characteristic turbulent time (integral turbulent time scale). It is derived from the used turbulence model. In the case of the (k, ε)-model it is given by $\tau_t = k/\varepsilon$, with ε measured in m^2/s^3.

In Eq.1 C_{EBU} is a model constant that either requires further modelling or is simply preset to a certain value using benchmark comparison calculations with experimental data. For COM3D,

this second approach was used, resulting in a C_{EBU} value of 6.0, which was found to give satisfactory results for a wide range of mixture parameters [6,7,8].
Note that for large k, i.e. $k^{1/2} >> S_L$, this extended model reduces to the standard EBU model since α will approach unity. For this reason, this model is regarded as an extension of the standard model towards flame regimes with a lower turbulence intensity, which usually corresponds to slow burning flames in lean mixtures.

The range of the combustion constant value, which is imposed by the model is limited by 1.0 from one side (this is a case of very high turbulence intensities $k^{1/2} >> S_L$) and by 5.4 from the other side (a theoretical case of zero turbulence intensity $k = 0$). In practical cases, the turbulence intensity k is always non-zero and is at least higher than 1000 m^2/s^2.
In this case a variation of the laminar flame speed from 0 to 3.5 m/s (laminar flame speed for stoichiometric H_2-air mixture) leads to the total change in α from 1.0 to 1.147. Therefore in practical cases the influence of the lower laminar flame speed in leaner mixtures will not exceed 15 % according to this model.

The subsequent two sections present the description of the experiment and its simulation performed in the frames of EU Fifth Framework Program Project HYCOM [e.g., 9].

Description of the mc043 experiment

The test mc043 was performed in the DRIVER tube [10,11], which is a cylindrical tube that can be equipped with obstacles to get a variable blockage ratio. In addition, a membrane can be introduced to subdivide the tube into sections with different concentrations.The internal diameter of both tube sections was 174 mm. A schematic of the experimental configuration is presented in Figure 1 and 2. In the corresponding series of experiments (tests in configuration 2) the combustion tube was separated into two sections of 6.04 m each, with different blockage ratio of the obstacles and different hydrogen concentrations (see table I). The two sections were separated by a diaphragm. The pressure required for membrane rupture was found to be about 660 Pa.

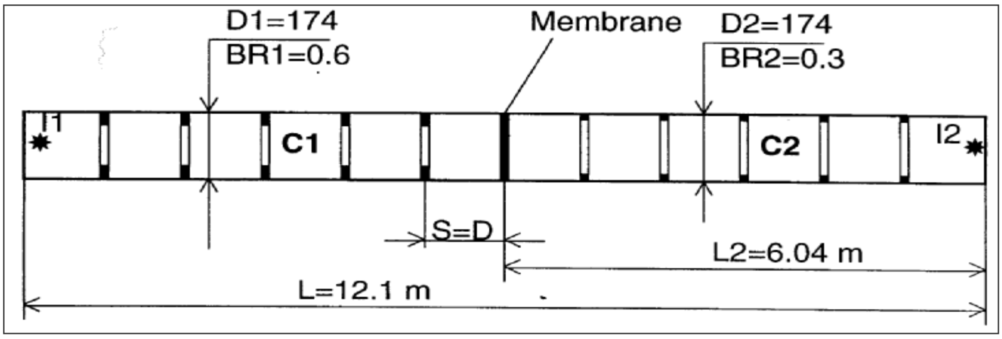


Figure 1. Scheme of configuration 2 for small-scale tests.

Test	C_1 (%)	Br_1	C_2 (%)	Br_2	ignition	regime
mc043	13	0.6	10	0.3	I1	fast / slow

Table I. Conditions of test mc043 (see Figure 1 for details).

In test mc043, the flame propagated from the 13% hydrogen mixture (where the sigma criterion was satisfied, which means flame acceleration cannot be excluded [12]) to the 10% hydrogen mixture (where the sigma criterion was not satisfied). The conditions of the experiment are shown in Table I. When the flame reached the lean mixture region, a transition from the fast choked flow regime to the slower subsonic flame was observed (see Fig. 3). In the first half of the tube, the flame accelerated along the first two meters and then reached a quasi-constant speed near 550 m/s, generating a high pressure wave with a peak pressure of nearly 10 bar, as shown in Fig.4. In the second half of the tube, the flame slowed down drastically, and the maximum pressures recorded by the transducers were significantly lower, except for the last transducer located near the end of the tube.

This test was chosen by the participating project partners for simulation as a good benchmarking example for the typical flame behaviour in non-uniform concentration fields as they generally develop in severe accidents. The flame propagation in lean mixtures has an unstable character and is typical for concentrations of about 10% and below. The simulation of such an experiment can therefore demonstrate the abilities of the code for the adequate predictions of the combustion characteristics in the region of lower concentrations.

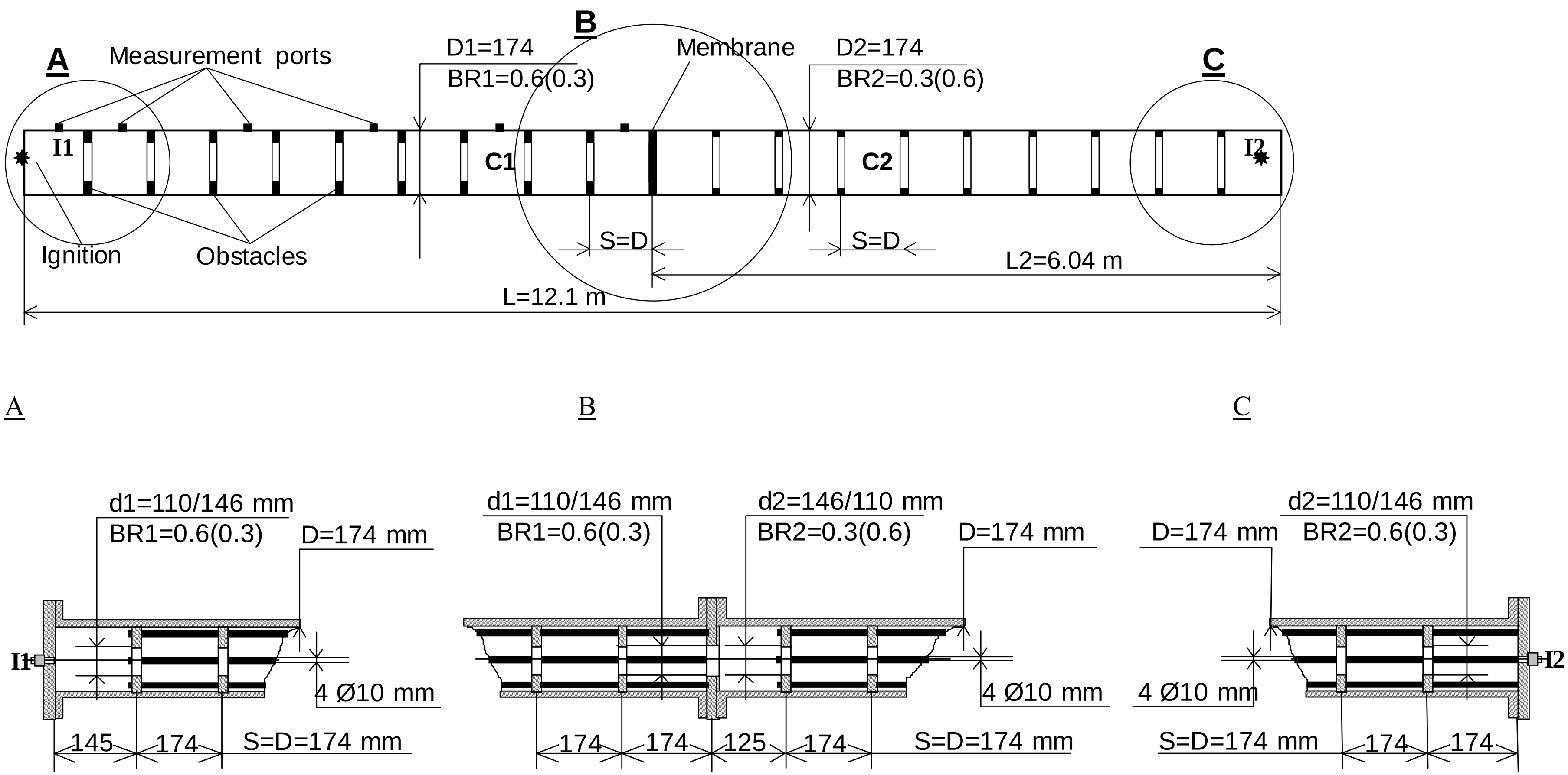
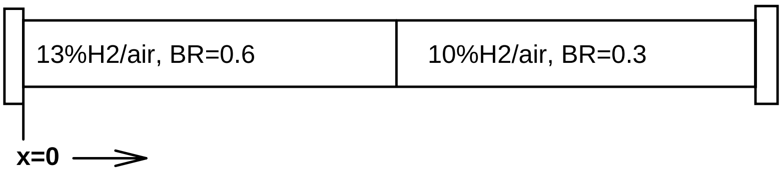


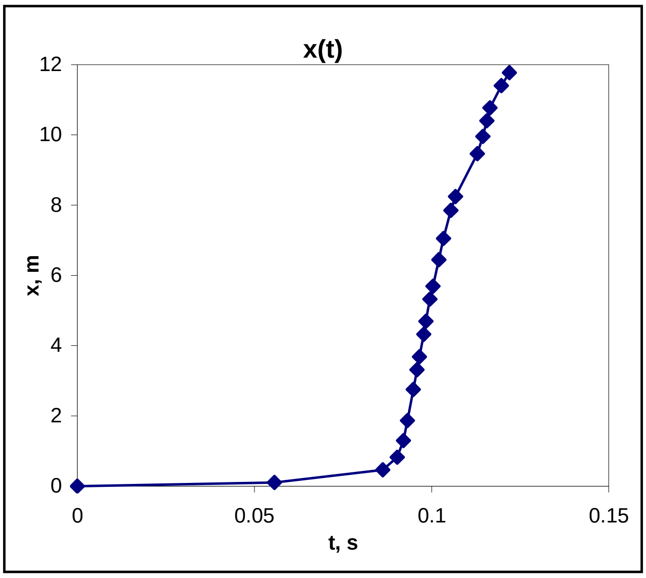
Figure 2. Schematic of the DRIVER combustion tube.

Experiment Mc043

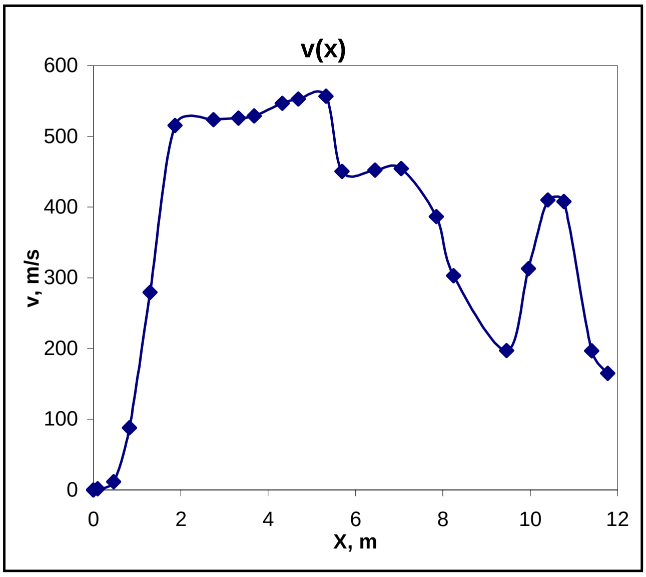
Configuration 2



Photodiode location x, m	Arrival time to,s	Local velocity v,m/s	
0	0	0	ignition
0.102	0.0557	1.83	
0.463	0.0862	12	
0.822	0.0903	88	
1.3	0.0920	280	
1.872	0.0931	515	
2.752	0.0948	524	
3.32	0.0959	526	
3.685	0.0966	529	
4.325	0.0977	547	
4.69	0.0984	553	
5.325	0.0995	557	
5.69	0.1004	451	
6.45	0.1020	452	
7.05	0.1034	455	
7.85	0.1054	386	
8.25	0.1067	303	
9.462	0.1129	197	
9.96	0.1145	313	
10.403	0.1156	410	
10.77	0.1165	408	
11.407	0.1197	197	
11.773	0.1219	165	

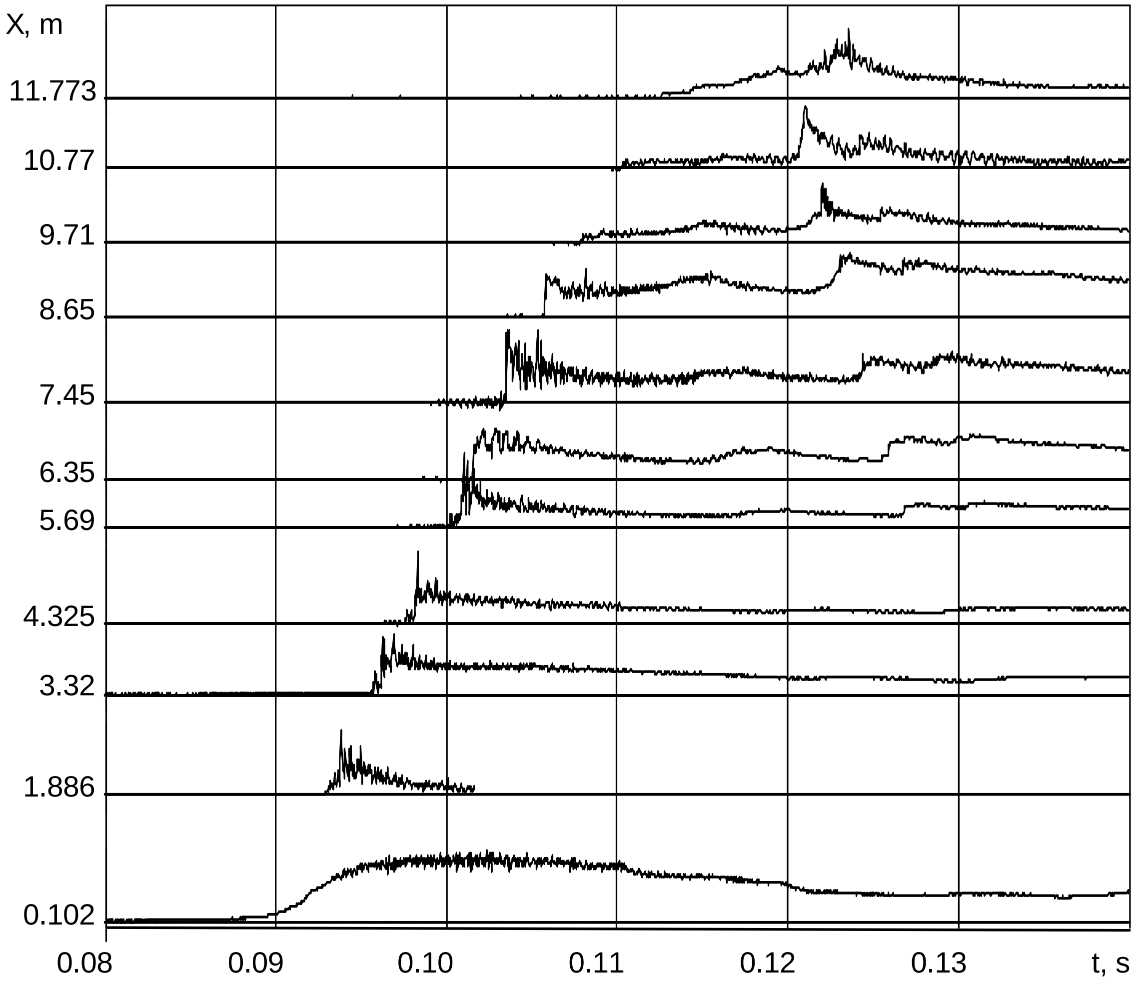


X-t diagram of explosion process



Local velocity versus distance

Figure 3. Experimental details and flame propagation characteristics in experiment mc043.



X, m	Pmax, atm	Transducer type
0.102	3.86	1
1.886	6.94	2
1.886	5.41	3
3.32	6.53	1
4.325	9.23	1
5.69	9.63	1
6.35	3.38	1
7.45	4.78	1
8.65	3.46	1
9.71	6.52	2
9.71	2.42	3
10.77	6.79	1
11.773	9.00	1

1 - piezoelectric transducers
2 - "fast" piezoresistive transducers
3 - "slow" piezoresistive transducers

Figure 4. X-t diagram (pressure histories) of the experiment mc043. Pressure transducers data.

Simulation of mc043 experiment

The results of the simulations of the test mc043 are reported in the following two sections. Flame speed and overpressure predictions are compared to the experimental results.

Flame speed

The spatial flame speed along the tube is extracted from the flame arrival times by the central differences method. It is plotted as a function of distance from the ignition location (at x=0) in Figure 5, in order to eliminate the shift in time between the different codes. By comparing the computed flame speeds with the experiment, it is possible to judge if the codes account correctly for the effect of hydrogen concentration and geometry on the flame acceleration or deceleration.

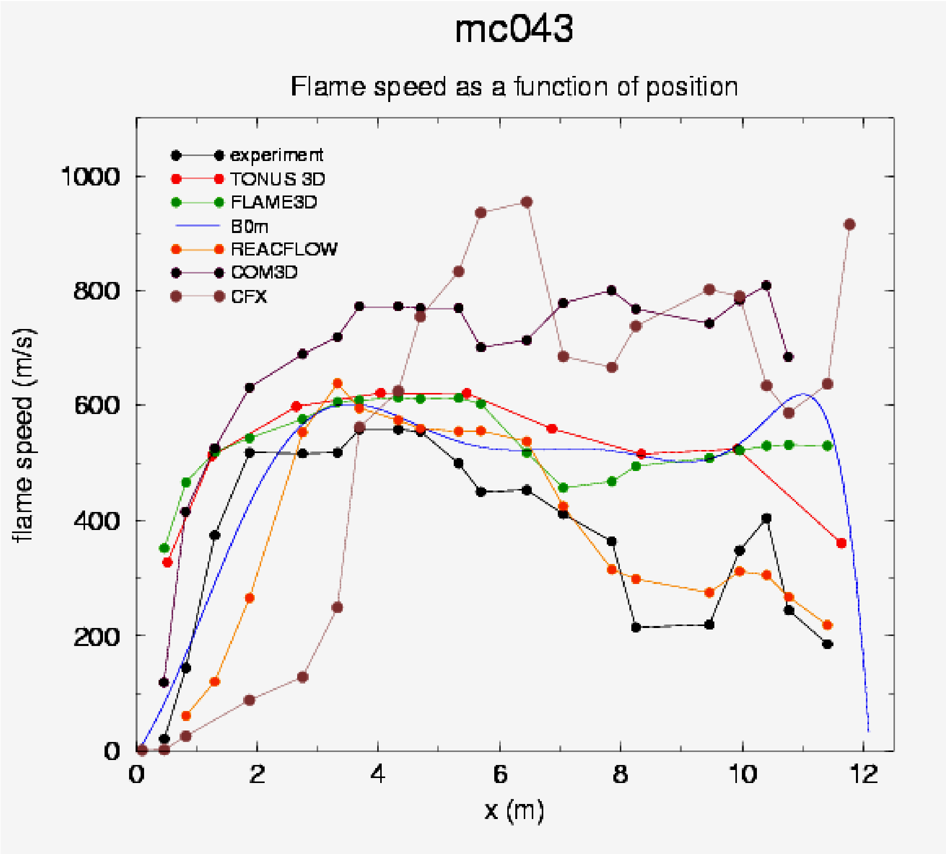


Figure 5. Comparison of flame speed as a function of distance for experiment mc043.

In the first half of the tube filled with the 13 % mixture, the flame accelerates up to about 550 m/s. This level of speed is predicted quite correctly by COM3D (first two columns of Table II), the maximal flame speed is slightly overestimated.

Table II. Comparison of flame speeds in experiment mc043.

	V_{max} in the first half of the tube [m/s]	Relative difference to experiment	V_{max} in the second half of the tube [m/s]	Relative difference to experiment
Experiment	558	-	404	-
Simulation	769	+37.8%	807	+99.8%

This fast combustion regime is established in the experiment after a distance of about 2 m, which corresponds to 11 obstacles. The code predicts this distance slightly longer and it predicts constantly higher flame velocities for a longer distance. The flame speed of 550 m/s is however reached earlier. These results are reflected in Table III. The criterion used to define the point at which the regime is established is a flame speed reaching 75% of the maximum flame speed in the 13% mixture.

Table III. Comparison of distances necessary to accelerate the flame in experiment mc043.

	Distance in first half at which $V>0.75V_{max}$ [m]	Relative difference to experiment
Experiment	1.49	-
Simulation	1.61	+8.05%

In the second half of the tube, the experimental results show a gradual deceleration of the flame down to 220 m/s, then a new acceleration of the flame up to 400 m/s and finally a strong deceleration of the flame near the end of the tube. In the last two columns of the Table II, the values of the local maxima in the second half of the tube (after eventual second acceleration) are compared. The COM3D code does not predict any noticeable decrease in the flame speed, the flame speed remains at the level achieved in the first half of the combustion tube with the value of about 800 m/s.

Overpressure

For the comparison of overpressures the following sensors were selected:
- 13% H2 section: 0.102 m (near ignition point), 4.325 m, and 5.69 m (close to transition);
- 10% H2 section: 6.35 m (close to transition), 8.65 m, and 11.77 m (near end of the tube).

These overpressures as a function of time are presented at the 6 locations in Figure 6. All the computed curves were shifted in time by a constant value: this value was chosen to meet the experimental pressure rise at the location x = 0.102 m.

In the first half of the tube, the general profiles of the pressure transients are well described by the code. At the first sensor located very close to the ignition point, the pressure rise is relatively slow, the maximal overpressure is not very high (3.86 bar) and oscillations exist but their amplitude remains limited in comparison to the pressure level. This is characteristic for a slow combustion regime with static pressure load on the walls. The code underestimates the maximal overpressure, but the discrepancy in the values is only about 5%, as can be seen in Table IV. The rate of the pressure drop after the pressure peak is well predicted by the code. The general agreement with the experiment is globally quite good.

Table IV. Comparison of maximal overpressures in the first half of the tube for experiment mc043.

Maximal overpressure (Pa)	x=0.102m	Relative difference to experiment	x=4.325m	Relative difference to experiment	x=5.69m	Relative difference to experiment
Experiment	3.86E5	-	9.23E5	-	9.63E5	-
Simulation	3.66E5	-5.2%	9.97E5	+8%	1.42E6	+47.5%

At the second transducer, located at x = 4.325 m, the fast combustion regime is fully established: the pressure transient is composed of several sharp pressure peaks; the highest of them being the first one that exceeds 9 bars (10 bars in absolute pressure). A lot of dynamic oscillations with higher amplitude than at the former sensor, probably due to transverse and longitudinal wave reflections in the tube, can be observed. The COM3D code captures very well the magnitude of the highest peak (8%). The start of the pressure rise happens somewhat earlier than in the experiment.

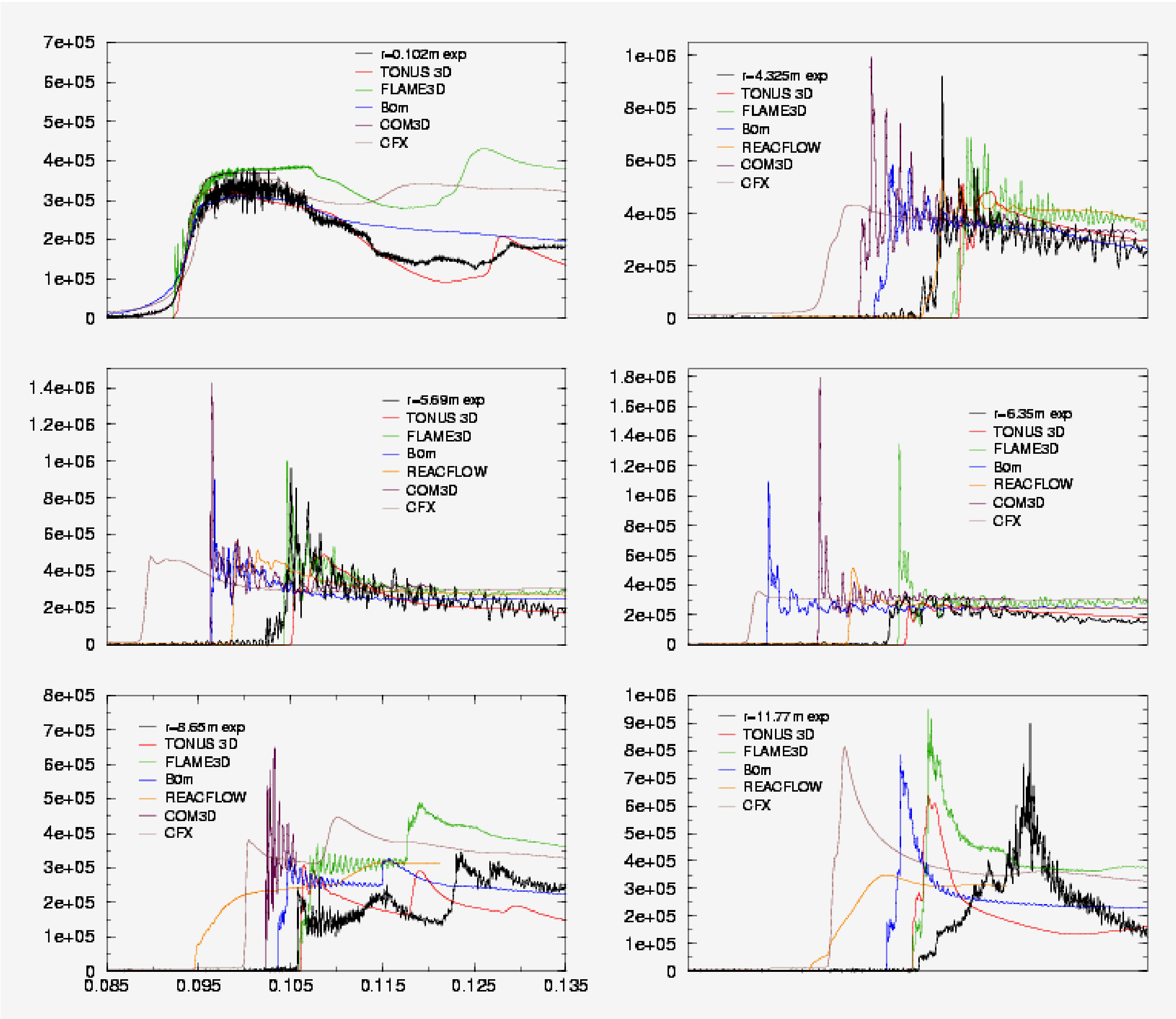


Figure 6. Comparison of pressure transients at different locations in experiment mc043. Pressure shown in Pa. Time scale is not shown.

At the third transducer, the profile of the pressure transient is very similar to the one observed at the second transducer. The value of the maximal overpressure is of the same order of magnitude but is overestimated by COM3D (see Table IV).

Table V. Comparison of maximal overpressures (in Pa) in the second half of the tube for experiment mc043.

	x = 6.35 [m]	Relative difference to experiment	x = 8.65 [m]	Relative difference to experiment	x = 11.77 [m]	Relative difference to experiment
Experiment	3.38E5	-	3.46E5	-	8.99E5	-
Simulation	1.79E6	+429.6%	6.51E5	+88.1%	-	-

In the second half of the tube, there is a considerable overestimation of both flame speed and the value of the peak pressures. The comparison of the maximal overpressures in the experiment and the calculation in this second half of the tube is presented in Table V.

At the fourth sensor (x = 6.35 m), the overpressure level drops drastically to less than 3.5 bar. Table V shows that the code still calculates pressure peaks equal or higher than the ones of the first part of the tube. The start of the pressure rise happens earlier than in the experiment. Similar conclusions can be drawn from the fifth sensor. No COM3D results are available for sensor 6.

Summary

The differences in the code predictions (particularly in the second half of the combustion tube) demonstrated again that non-uniform mixtures are still a challenge for numerical simulations, especially when they are accompanied by a change in the combustion regime (fast to slow deflagration in the case of mc043), but also that a conservative simulation is possible with COM3D.

From the point of view of safety analysis the flame velocity of the combustion process is the most important parameter to describe the whole explosion event. In most cases the flame speed defines the pressure evolution and thus the resulting structural loads on the confining constructions. Therefore a comparison of the experimental data and corresponding simulations has to be made in terms of flame velocities. Conclusions about code conservatism are justified if the predicted values of flame speed are not below the values observed in the experiment.

The comparison of the experiment mc043 and its simulation demonstrated that in the area of lean mixtures (10% vol. H_2) the COM3D code predicts definitely higher flame speeds. In case of leaner mixtures than studied here (H_2 concentration below 10%) and different combustion processes, code conservatism can be expected due to the following reasons:

- in the whole range of concentrations the same combustion model constant defining chemical interaction is used. For the EBU models the general tendency consists in reduction of combustion constant with the reduction of reactivity (i.e., H_2 concentration) of the system. Since it was shown that for 10% H_2-air mixture the code predicts higher combustion velocities than experimentally observed, it can be expected that for leaner mixtures (with concentration below 10%), the degree of conservatism will increase.

- heat losses (which become more important for slower processes, as e.g., at initial stages of FA or during combustion in leaner mixtures) are currently not taken into account in the COM3D modelling. This fact can lead only to overestimation of flame velocities and with the decrease of characteristic rate of the combustion process the degree of overestimation has to increase. In the modelled case the combustion velocities are relatively high and consequently an influence of heat loses is negligible. Therefore, taking into account these facts and that even in the modelled case the calculated velocities were higher than experimental, it can be expected that for leaner mixtures (with concentration below 10%), the degree of conservatism of the code predictions can only increase.

These justifications can be considered as a good basis for the confirmation of the code conservatism in evaluation of blast loads resulting from the combustion processes in the lean mixtures. Continuation of the validation work at the same time with the development of the advanced combustion models were planned and are under way for the challenging situation of lean mixtures.

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