MODELING OF HYDROGEN FLAME DYNAMICS IN NARROW GAP WITH BENDABLE WALLS

Kotchourko, A.[1], Lelyakin, A.[1], and Jordan, T.[1]
[1] IKET, Karlsruhe Institute of Technology, Kaiserstraße 12, Karlsruhe, 76131, Germany, alexei.kotchourko@kit.edu

ABSTRACT

A concept of volume porosity together with model of moving walls were elaborated and implemented into the COM3D code. Additionally to that a support of real-time data exchange with finite-element code ABAQUS - © Dassault Systèmes provided possibility to perform simulations of the gas-dynamic simultaneously with geometrical adaptation of environmental conditions. Based on the data obtained in the KIT combustion experiments in narrow gaps [1], the authors performed a series of the simulation on the combustion in the corresponding conditions. Obtained numerical results demonstrated good agreement with the observed experimental data. These data were also compared with those obtained in the simulation without wall bending, where simulation showed considerably different combustion regime. Application of the developed technique allows to obtain results unreachable without accounting on wall displacements, which demonstrates massive over-estimation of the pressures observed during flame propagation.

1.0 INTRODUCTION

Problem of the possible high-speed combustion processes in the modern appliances, such as e.g., fuel cells, has specific features connected with peculiarities of their internals. For example, a number of gaps or narrows in the solid parts of the stack surrounded by thin metal walls can be easily found in the typical fuel cell. In case when ignitions occurs and the combustion propagates in such gaps, the degree of the possible wall bending can critically affect the combustion regime, and an adequate accounting of such effects can appear to be decisive for safety analysis.

With the aim to enhance capabilities of the COM3D code to predict combustion regime and process characteristic in different geometrical conditions, a concept of volume porosity (see, e.g., [2]) together with a model of moving walls were elaborated and implemented into the code. These new attainments allowed to realize support of real-time data exchange with finite-element analysis code ABAQUS - © Dassault Systèmes, which provides a new possibility to perform simulations of the combustion gas-dynamic processes simultaneously with possible adaptation of the changing geometrical and thermo-dynamical environmental conditions.

The current implementation of the COM3D and ABAQUS two-way coupling provides exchange of information between these two codes on every time step and on the pre-defined set of nodes known for both codes. From COM3D, the information on the 3D force acting on each node is transferred, and in the opposite direction from ABAQUS, the 3D displacement vector and 3D velocity vector are transferred. This allows to adjust COM3D simulation geometry immediately when it modifies.

Based on the data obtained in the recently performed experiments on combustion and flame acceleration in the narrow gap [1], the authors performed a series of the simulations on the combustion in the conditions corresponding to the experimental ones. From these series of the simulations, one simulation, which was performed with accounting for the wall bending and another one without accounting of wall bending, will be discussed.

2.0 DESCRIPTION OF THE VALIDATION EXPERIMENT

The experiment were conducted in Karlsruhe Institute of Technology in Germany. The experiments were made with the idea to study possible flame acceleration and DDT in stoichiometric hydrogen-air mixtures in a thin layer geometry.

The experimental set up is a set of PVC frames covered from both sides by Plexiglas walls (see Figure 1). Each frame is 1000 mm long and 350 mm wide with internal cut of 900 mm long and 200 mm wide. The Plexiglas covers has the same outer dimension 1000 mm x 350 mm and both are 12 mm thick. In the referenced experiment, thickness of the PVC frames was 8 mm.

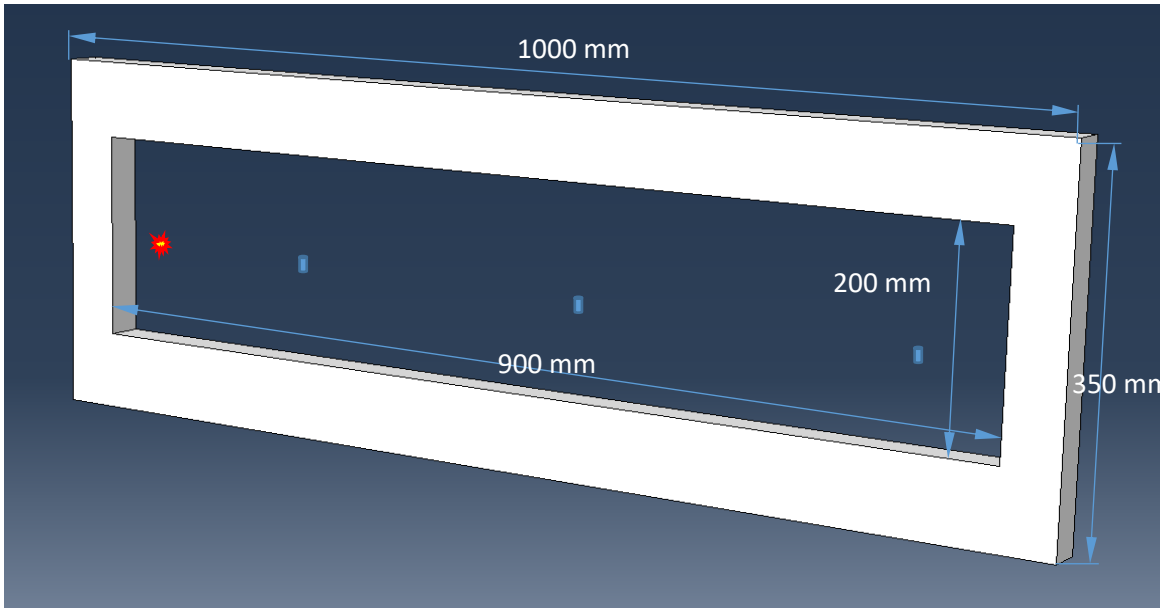

Figure 1. Schematic of the experimental combustion channel. Plexiglas panels are not presented. An ignition position is shown with red spot; the positions of the pressure transducers are shown with blue cylinders.

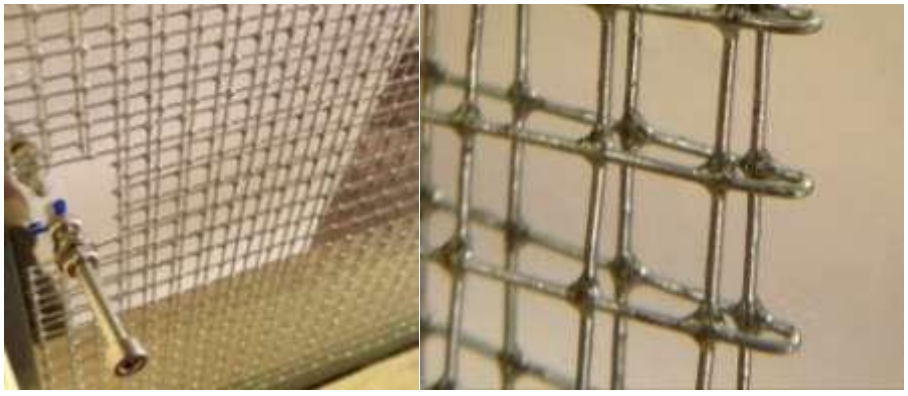

Figure 2. Two metal wire grids of 6.5 x 6.5 x 0.6 mm located inside volume with combustible mixture. Figure courtesy M. Kuznetsov [1].

The mixture was ignited by ignitor located in the middle of internal channel and 10 mm apart from the rare wall. There were pressure sensors installed at the centerline with coordinates from internal volume rear wall equal to 150 mm (P1), 500 mm (P2), and 850 mm (P3). The pressure transducers are mounted to the sidewall without contact with window walls to keep the signal undisturbed. To promote fast combustion inside the combustion volume two metal wire grids were located. The grids were fabricated from a wire 0.6 mm diameter, with a mesh size of 6.5 mm x 6.5 mm (Figure 2).

The experiment was carried out for stoichiometry hydrogen-air mixture at ambient conditions (~20 °C; ~1000 bar). Obtained results on the obtained pressure and displacement of the Plexiglas wall is shown in Figure 3.

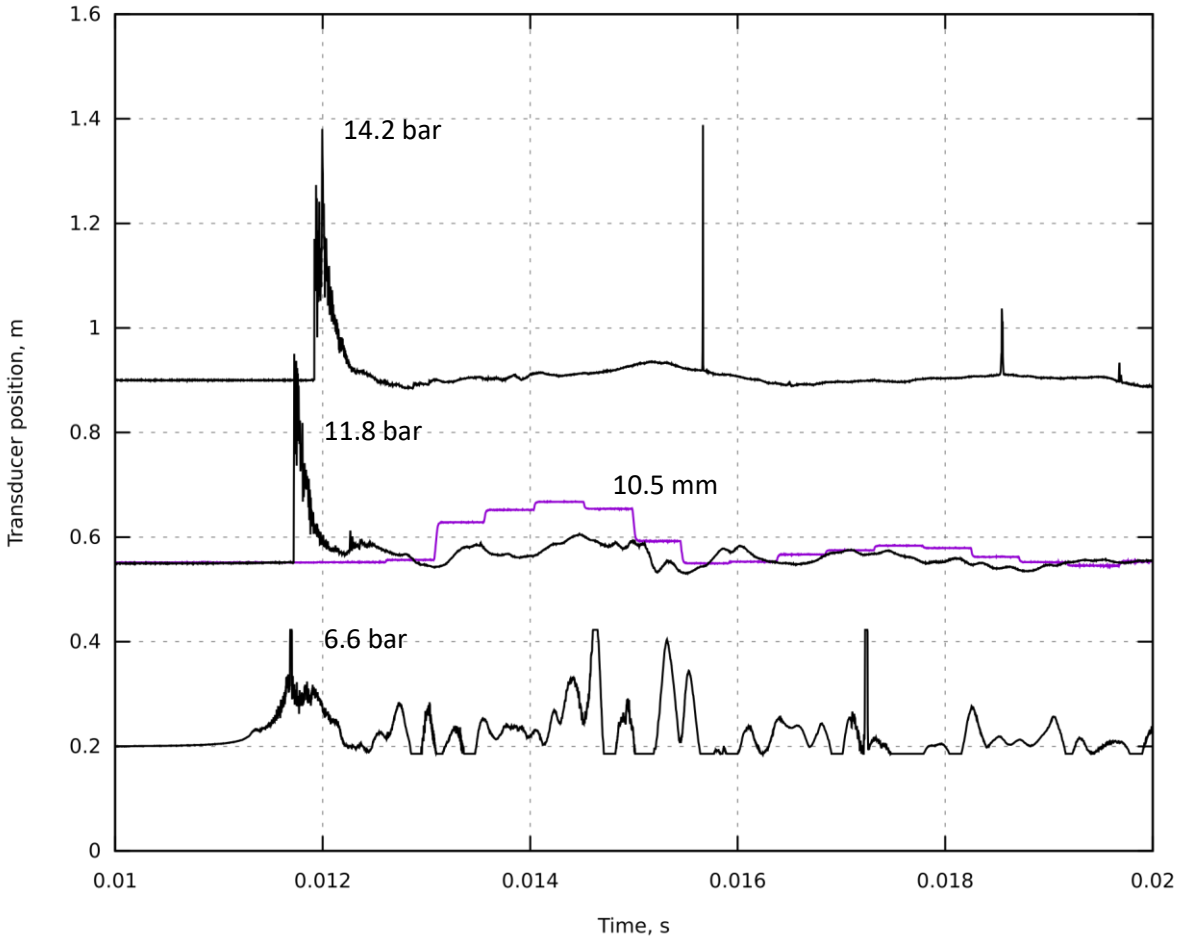

Figure 3. X-t diagram showing pressure signal (black) at different locations along the combustion chamber and the measured wall displacement (purple).

3.0 DESCRIPTION OF THE MODEL

The current implementation of the COM3D and ABAQUS two-way coupling provides exchange of information between these two codes on every time step and on the pre-defined set of nodes known for both codes. From COM3D, the information on the 3D force acting on each node is transferred, and in the opposite direction from ABAQUS, the 3D displacement vector and 3D velocity vector are transferred.

Thus, the geometry model in both codes should be high degree comparable, especially in the areas where data transfer is performed. The geometry model for COM3D must include wall cells as well as in the ABAQUS code.

3.1 Geometry model

The total calculation domain (see Figure 4) has 1000 x 350 x 32 (totally 11 200 000) cubic cells of 1 mm cell side size. Corresponding to the experimental set up, internal area filled with gas mixture was 900 x 200 x 8 (totally 1 440 000) cells.

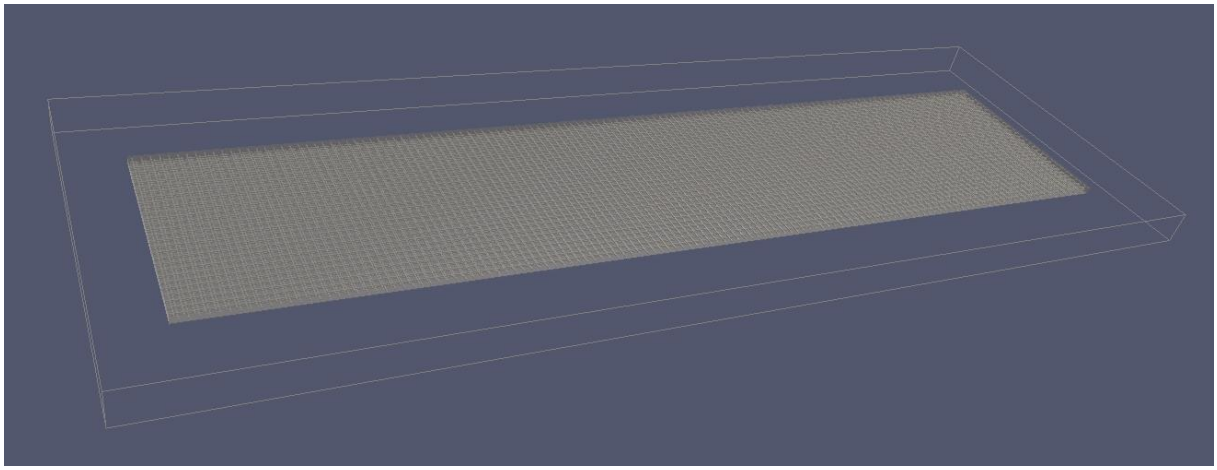

Figure 4. Overview of the geometry model. Calculation mesh is not shown. Model of the wire frame can be seen in the internal section.

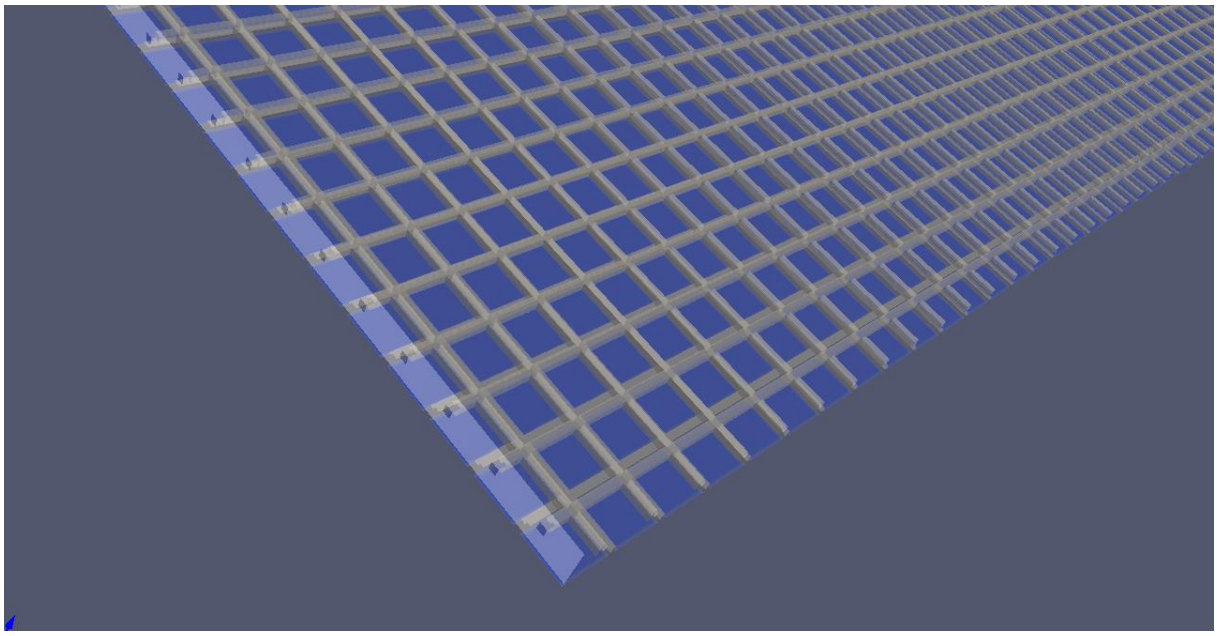

Figure 5. Details of the internal section with two grids inside.

Inside combustion volume, two wire grids (Figure 4, Figure 5) with the blockage ratio calculated in the transverse direction (TBR) equal to 0.26 were located. In comparison with the TBR from the experiment

equal to 0.18, it has somewhat higher value, which is determined by calculation mesh sizes. Each grid was separated from the chamber wall by gas gap in two cells and the wire cross section has 1 x 1 mm.

The blockage ratio calculated in the longitudinal direction (LBR) for experimental conditions can be evaluated being in the range 0.15 ÷ 0.3. Higher value resulted from assumption of double wire cross section due to wire superimposing in perpendicular directions. The LBR in the numerical geometry model is equal to 0.25.

3.2 Governing equations

The COM3D code solves set of the Reynolds-Averaged Navier-Stokes (RANS) conservation equations for mass, momentum, energy and species.

$$(\rho)_t + (\rho u_j)_{x_j} = 0\,, \tag{1}$$

$$(\rho u_j)_t + (\rho u_i u_j)_{x_j} = \rho g_j - p_{x_j} + M_{ij,x_j}\,, \tag{2}$$

$$(\rho e)_t + ((\rho e + p)u_j)_{x_j} = \rho g_j u_j + u_i M_{ij,x_j} + (\frac{\mu}{C_h}(e - \frac{1}{2}u_i u_j + \frac{p}{\rho})_{x_j})_{x_j} + B + \rho\varepsilon\,, \tag{3}$$

$$(\rho Y_\alpha)_t + (\rho Y_\alpha u_j)_{x_j} = (\frac{\mu}{C_h} Y_{\alpha,x_j})_{x_j} + \overline{\omega}_\alpha\,, \tag{4}$$

$$e = \sum_{\alpha=1}^{N} \frac{Y_\alpha}{\mu_\alpha}(h_\alpha + \Delta h_\alpha^0 - RT) + \frac{1}{2}u_j u_j\,, \tag{5}$$

$$Y_\alpha = \frac{\rho_\alpha}{\rho}\,,$$

with standard *k*-ε model, where

$$M_{ij} = -\frac{2}{3}\delta_{ij}(\overline{\rho}\overline{k} + \overline{\mu}\overline{u}_{r,x_r}) + \overline{\mu}(\overline{u}_{i,x_j} + \overline{u}_{j,x_i})\,, \tag{6}$$

$$S = \overline{u}_{i,x_j} M_{ij} - B\,, \tag{7}$$

$$B = \frac{\overline{\mu}}{C_\rho}\frac{1}{\overline{\rho}^2}\overline{\rho}_{x_r}\overline{p}_{x_r}\,. \tag{8}$$

and with transport equations for k and ε

$$(\overline{\rho}\overline{k})_t + (\overline{\rho}\overline{k}\overline{u}_j)_{x_j} = S - \overline{\rho}\overline{\varepsilon} + (\frac{\overline{\mu}}{C_k}\overline{k}_{x_j})_{x_j}\,, \tag{9}$$

$$(\overline{\rho}\overline{\varepsilon})_t + (\overline{\rho}\overline{\varepsilon}\overline{u}_j)_{x_j} = \frac{\overline{\varepsilon}}{\overline{k}}\left[C_1 S - C_2\overline{\rho}\overline{\varepsilon}\right] + (\frac{\overline{\mu}}{C_{f_\alpha}}\overline{\varepsilon}_{x_j})_{x_j}\,, \tag{10}$$

where

$$\bar{\mu}_t = \bar{\mu} + C_\mu \frac{\bar{k}^2}{\bar{\varepsilon}} .$$

For ignition and flame propagation modelling, combustion model KYLCOM was used. KYLCOM model provides propagation of the flame with specified velocity, defined by one of turbulent flame velocity expressions available [3]. In the current work, the following expression for the evaluation of the turbulent combustion speed (see [4, 5]) was used

$$S_{t_1} = 1.53\,(Ka\,Le)^{-0.3}\,;\; S_{t_2} = S_L(1 + 0.7\left(\frac{u'}{S_L}\right)^{\frac{1}{2}} \quad \left(\frac{L}{\delta}\right)^{\frac{1}{4}};\; S_t = \min(S_{t_1}, S_{t_2})\,. \tag{11}$$

3.3 Embedded boundaries

For the accounting of wall movement, the concept of 'moving embedded boundaries' was implemented in the COM3D code. There are few different approaches to realize moving boundaries (see e.g., [6, 7]), in COM3D, in the contrast, it is assumed that the effective cell volume can be changed during simulation depending on the force applied to the cell boundary and the material of the cell. This is reached allowing effective (or real) boundary to move inside the cell, i.e., a cell can be partially filled with gas and partially with solid (Figure 6), and the boundary between them becomes such 'embedded' boundary.

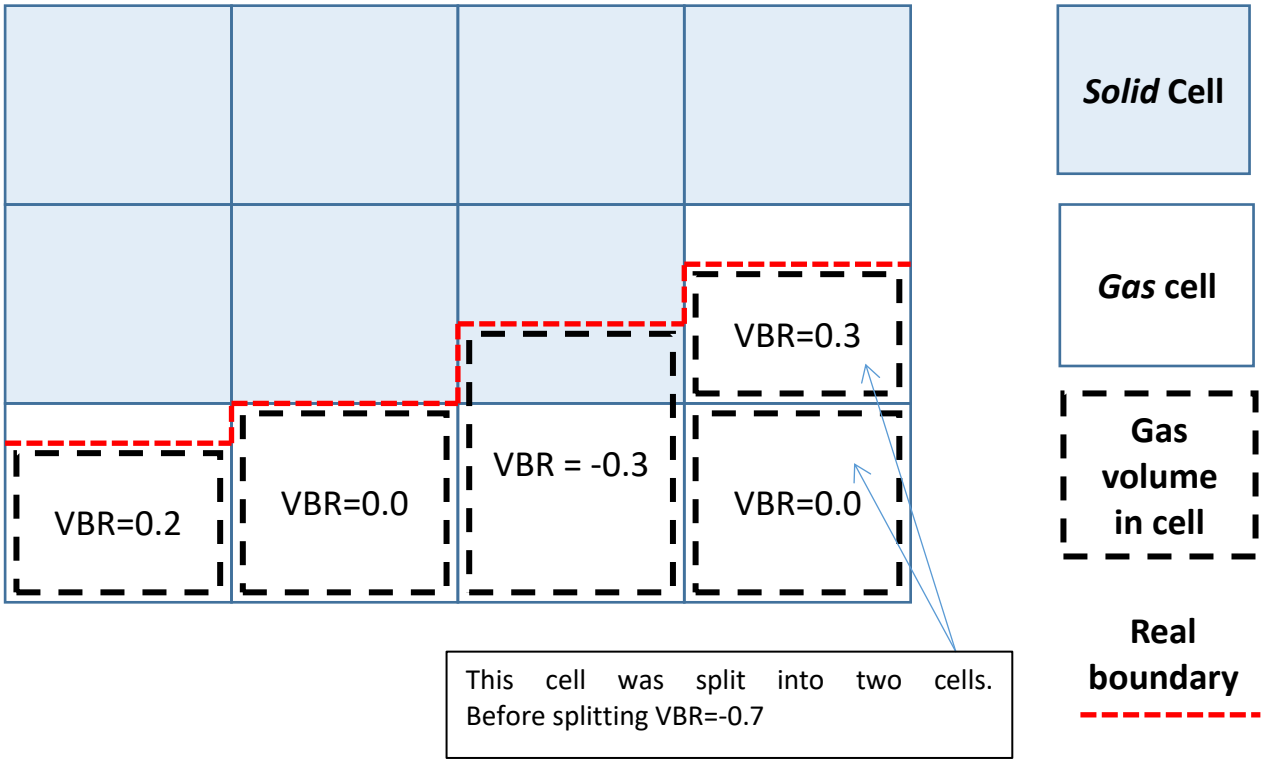

Figure 6. Definition of volume blockage ratio (VBR) for different configurations.

In general the embedded boundary can have an arbitrary degree of complexity, though for efficiency reason in the current version of COM3D code, the simplest approach is used: in the 'embedded' cell there may be at most one face that can move. This face can move only in direction normal to this face. As soon as the model takes into account only the one-dimensional movements, which are directed along

the normal to the moving boundary, only components normal to the surface of exchanged fields are participated in the data transfer between codes.

When face displacement exceeds the size of a cell, the calculating mesh is re-generated, otherwise accounting of the wall dislocation is performed using sub-grid model of the 'embedded' boundary. 'Embedded' boundary model includes control of the calculation cell fraction occupied by gas/solid material, and corresponding correction of fluxes through the cell boundaries and field parameters inside the cell.

To represent position of embedded boundary additional property of cell was introduced: volume blockage ratio (VBR). This property shows which part of volume of a cell is blocked by wall. Default value of zero for this property represents the case of undisturbed cell. When boundary moves inside cell and cell becomes rather small in one direction, than effective cell size and corresponding stability limits for time step can be too strict.

To prevent time step limitation we allow for embedded boundary not only to move into cell, but also to extend to outside. That means that our 'blockage ratio' can be not only positive, but also negative. Allowed range of values is from -0.5 to+0.5.

Here positive values represent embedded boundary that is moved into the cell. Negative values represent cell expanded to outside. Blockage ratio multiplied by cell size represents displacement of boundary. Here positive sign of displacement is inside gas, negative - outside.

If during simulation blockage ratio goes outside of allowed limit [-0.5, +0.5] than decision is taken either to split this cell into two cells, or to combine this cell with the neighboring cell.

Modified solution procedure takes into account the fact that amount of gas in the cell is changed due to blockage of that cell. Another modification takes into account the changed area of cell face. Currently area of cell face is estimated on the basis of blockage ratio of two cells that this face is dividing and on the basis of information on boundary conditions in these cells.

To achieve second order of approximation of solution it is necessary not only to take into account the blockage ratio of cells, but also changes of that blockage during time step. To achieve that additional property was introduced: rate of change of blockage ratio. As blockage ratio is dimensionless, the rate of its change is measured in inverse seconds. Actual velocity of wall motion is that rate multiplied by cell size.

During co-simulation COM3D receives from ABAQUS not only displacements, but also velocities of interface between gas and solid. Without co-simulation the rate of change of blockage ratio remains constant thus representing a wall moving with constant velocity.

4.0 SIMULATIONS AND RESULTS

The combustion was modelled using standard COM3D combustion model KYLCOM. Two simulations were performed for the same conditions: i) with accounting of the wall bending, i.e., in the co-simulation session with ABAQUS; ii) without accounting of the wall bending.

Initial combustion process was slow up to 4 ms of the simulation time after ignition, and no visible displacement of the walls was observed. From 4^{th} ms to 5^{th} ms, strong flame acceleration was observed and by the end of 5^{th} ms all hydrogen has been burned out. Figure 7, showing resulting hydrogen concentration, demonstrates that only small part of the volume near wall still has residual amount of hydrogen. Figure 8 and Figure 9 demonstrate that by the end of combustion, the highest displacement

is located still in the rear part of the volume, which is connected with noticeable inertia of the combustion chamber walls.

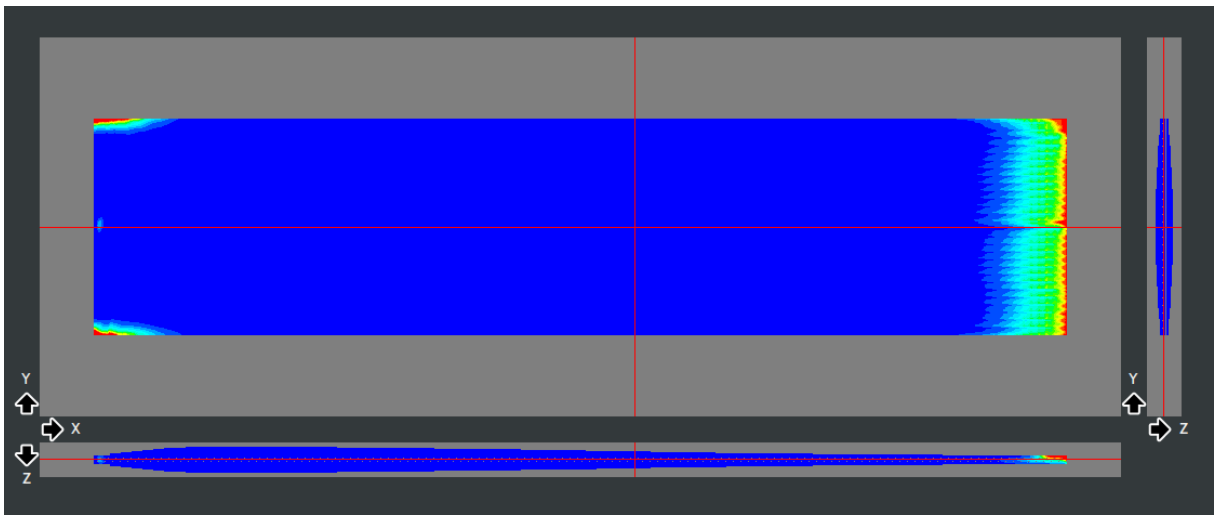

Figure 7. Hydrogen distribution at the end of combustion, which corresponds to 5 ms simulation time after ignition.

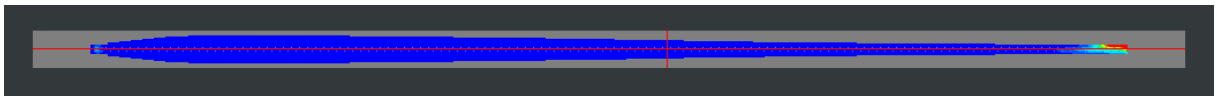

Figure 8. Plexiglas wall profile at the end of strong flame acceleration in the second half of the facility in COM3D. Time 5 ms simulation time after ignition.

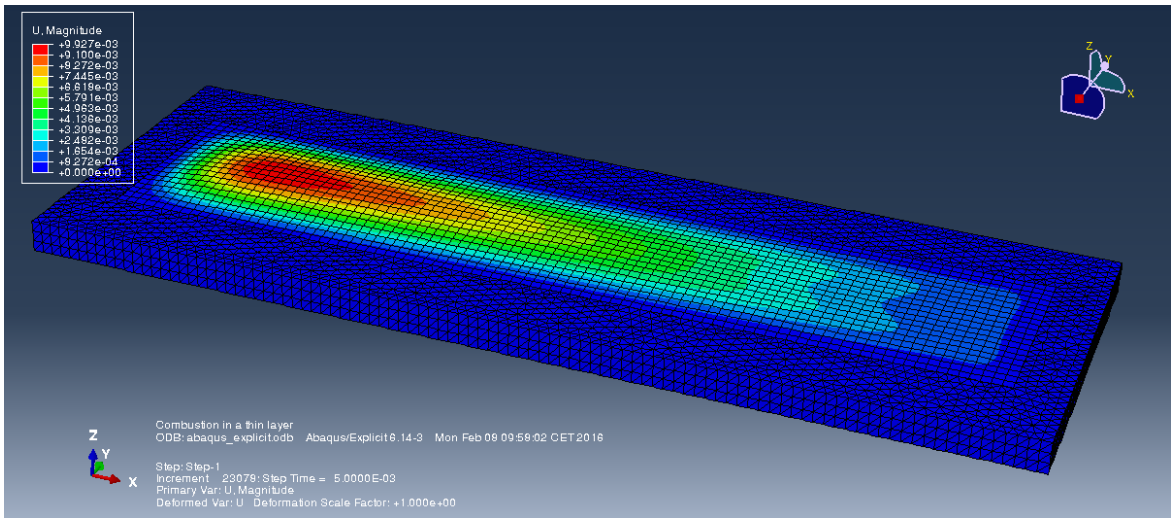

Figure 9. Wall displacement at the end of strong flame acceleration in the second half of the facility in ABAQUS. Time 5 ms simulation time after ignition.

After approximately 2 ms the wall configuration obtains more symmetric form due to the curvature propagation toward front wall (Figure 10). The timing of the maximum wall displacement approximately corresponds to the maximum observed in the experiment as it is shown in Figure 3 with purple curve.

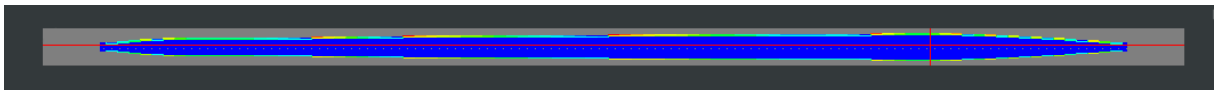

Figure 10. Plexiglas wall profile 2 ms after end of combustion process.

When pressure inside combustion section is near ambient atmospheric pressure and only relatively week acoustic waves propagates forth and back along the volume, the wall displacement distribution has a specific form with two 'hills' near volume ends appears (Figure 11). These 'hills' grow due to local pressure growth near the wave reflections from the volume ends.

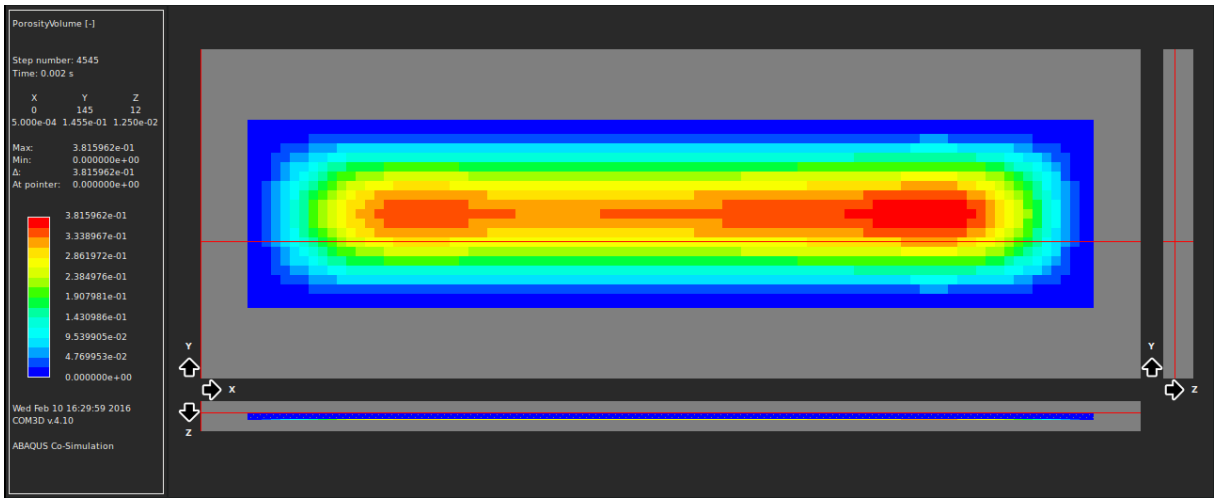

Figure 11. Wall displacement distribution by nearly uniform overpressure with acoustic waves.

Comparison of the simulation results with the results obtained in the experiments, shown in Figure 12, demonstrates good agreement in the character of the combustion process. Convergence of the leading wave amplitude, character of the flame acceleration, and flame speed in all stages of combustion, confirms the capability of the developed technique for adequate reproduction of the phenomena under consideration.

In the simulation without accounting for the possible wall bending, propagation of the flame head had the character similar to those observed in the first simulation. Take into account the fact that in both simulation the head propagates in still narrow channel, since the channel broadens only few millisecond later, the conditions at the head are essentially analogous. However, the pressure after shock differs considerably, and for the narrow channel the pressure exceeds the pressure in the broadened channel almost three times (Figure 13). This can result in the considerably greater impulse, and thus can be potentially much more dangerous.

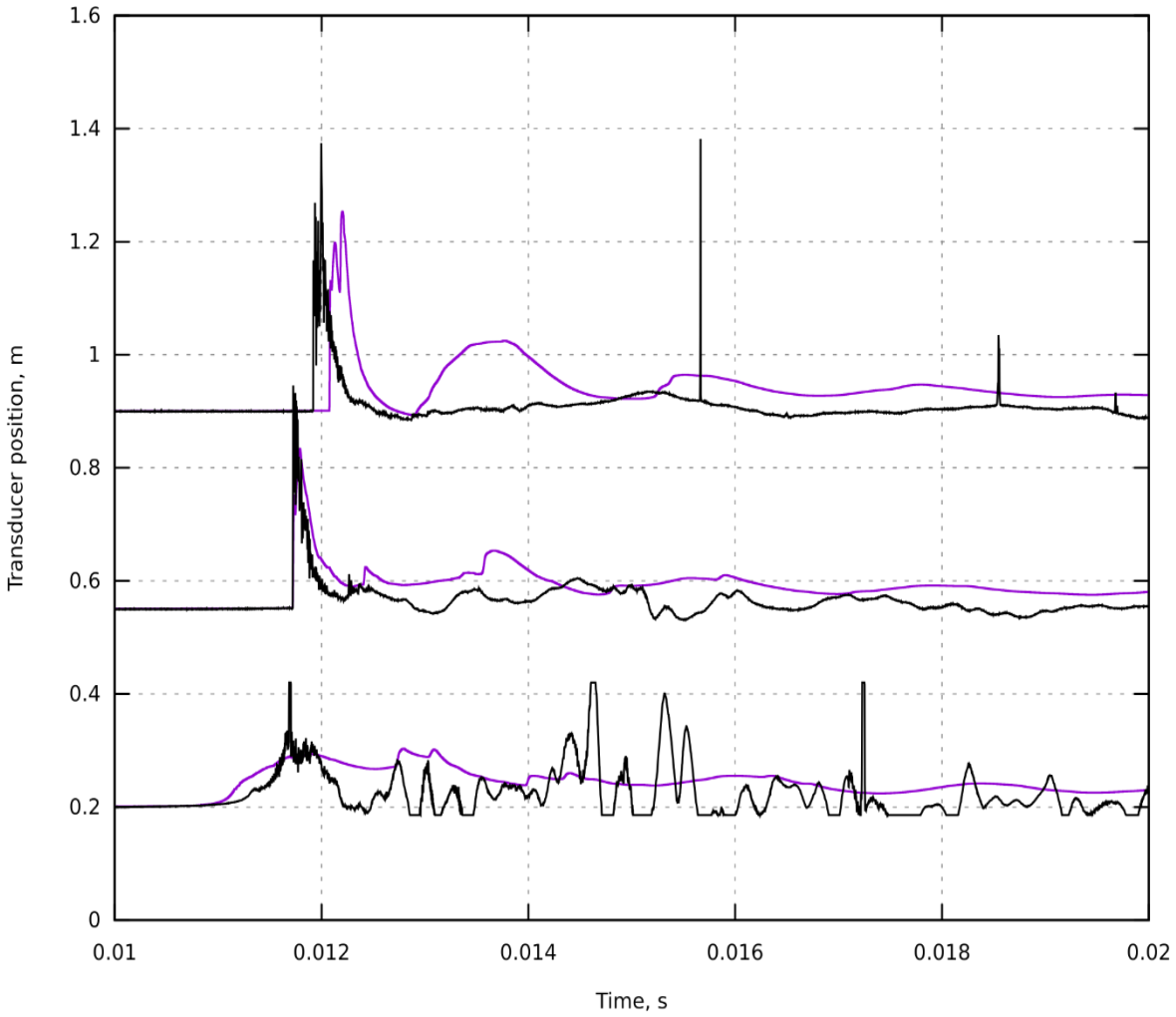

Figure 12. Comparison of the experimental results and simulations as X-t diagram. Records of the three pressure transducers are shown. The horizontal axis corresponds to time in seconds, vertical axis denotes position of the transducers. Experimental data shown in black, simulation in purple.

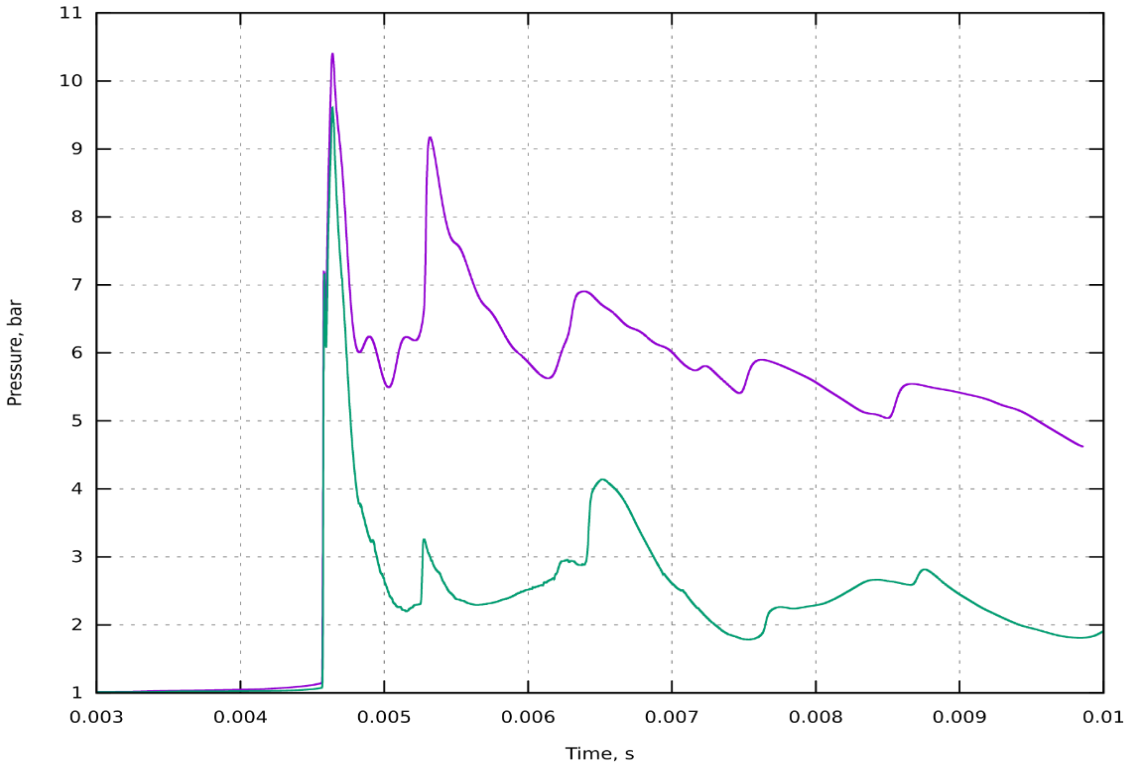

Figure 13. Comparison of the pressure records of gauge P1 (500 mm) in two simulations. Green line shows pressure dynamics in the co-simulation with ABAQUS, purple curve shows pressure record in the simulation with accounting of wall bending. Shock fronts were shifted for convenience.

5.0 CONCLUSION

Recently developed and implemented in COM3D code model of 'embedded boundaries', utilizing porosity idea, allowed to realize a possibility of real-time data exchange with finite-element code ABAQUS - © Dassault Systèmes. High quality finite-element analysis performed by ABAQUS based on the data from gas-dynamic data from COM3D gives new capabilities to carry out simulations with modifiable geometrical environment.

Using new capabilities, two validating simulations based on the experimental data were performed and demonstrated an importance of the accounting of the possible geometry changes. Obtained in the co-simulation with ABAQUS session, numerical results demonstrated good agreement with the observed experimental data.

Comparison of these pressure records with those obtained in the simulation without wall bending showed considerably different combustion parameters. Application of the developed technique allows to obtain results unreachable without accounting of the geometry modifications. Comparison of the experimental results and data from simulation with and without displacement demonstrated massive over-estimation of the pressures observed during flame propagation.

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