MODELING OF TUBE DEFORMATION AND FAILURE UNDER CONDITIONS OF HYDROGEN DETONATION

Kotchourko, A.[1], Lelyakin, A.[1], Offermanns S.[2] and Jordan, T.[1]
[1] ITES, Karlsruhe Institute of Technology, Kaiserstraße 12, Karlsruhe, 76131, Germany, alexei.kotchourko@kit.edu
[2] MPA, University of Stuttgart, Pfaffenwaldring 32, D-70569 Stuttgart, Germany

ABSTRACT

In case of accidental conditions involving high-speed hydrogen combustion, the considerable pressure and thermal loads could result in substantial deformation and/or destruction of the industrial appliances. Accounting of such effects in the safety analysis with CFD tools can provide critical information on the design and construction of the sensitive appliances' elements. The current paper presents the development and the implementation of a new 3D-technique, which makes possible to perform simulations of the gas-dynamic processes simultaneously with adaptation of the geometry of complex configurations. Using the data obtained in the experiments on the flame acceleration and DDT in the tubes of industrial arrangements performed in MPA and KIT, the authors performed a series of the combustion simulations corresponding to the experimental conditions. The combustion gas-dynamics was simulated using COM3D code and the tube wall material behavior was modelled using finite-element code ABAQUS - © Dassault Systèmes with real-time data exchange between the codes. Obtained numerical results demonstrated good agreement with the observed experimental data on both pressure dynamics and tube deformation history.

1.0 INTRODUCTION

The possible high-speed combustion processes in the industrial appliances, which typically include tubes or channels, where DDT processes are highly possible, can lead to the considerable deformation or even destruction of such system parts. The deformation/failure of the tubes/channels can critically affect the expected pressure loads on the walls and parts, therefore a proper consideration of such effects can be decisive by the appliances' design and construction. (see, e.g., [1]).

In the frames of general COM3D code [2] improvement and supplemented model development, a concept of sub-grid volume blockage was elaborated and implemented into the code. The model introduces 'joint boundary surface' describing exact position of the boundary through the regular rectangular grid. The 'surface' consists of the triangular elements which can relocate in time while forming continuous non-breakable shell. These accomplishments allowed to expand existed before 2D-algorithm to new 3D-technique, which makes possible to perform simulations of the gas-dynamic processes simultaneously with highly accurate adaptation of the geometry of complex configurations.

Based on the data obtained in the experiments on the flame acceleration and DDT in the tubes of industrial arrangements performed in Material Testing Institute of Stuttgart University and ProScience GmbH, the authors performed a series of the combustion simulations corresponding to the experimental conditions. The simulations were performed with COM3D code using finite-element analysis code ABAQUS - © Dassault Systèmes for tube walls deformation modeling in the course of the co-simulation sessions, allowing data exchange through network interface at every time step. Obtained numerical results demonstrated good agreement with the observed experimental data on both pressure dynamics and tube deformation history. These data also allowed to reproduce sequence of events leading to the dangerous deformations and to the tube failures. Utilization of the developed technique allows to predict the situations critical for the safety aspects of the considered accident scenarios.

2.0 DESCRIPTION OF THE EXPERIMENTS

The experiments were performed in the frames of the research program of the study of austenitic tube behavior under pressure load [3, 4]. All three experiments which were analyzed were performed in combustion tubes of different configurations. The tubes were equipped with pressure and displacement transducers. In the experiments, oxyhydrogen (mixture of two parts H_2 with one part of O_2) with different addition of nitrogen was used. In all experiments initial pressure was 70 bar, and temperature was taken 298.15 K. The far end of the tube was equipped with a rupture membrane.

Test V80E3:

- mixture 80% oxyhydrogen and 20% nitrogen;
- tube parameters
  - wall thickness 6.02 mm;
  - tube length 3817 mm;
  - outer tube diameter 114.3 mm.

Test V100G2:

- mixture 100% oxyhydrogen
- tube parameters:
  - wall thickness 8.56 mm;
  - tube length 3240 mm;
  - outer tube diameter 114.3 mm;
  - pressure transducer positions: 0.56 m, 0.71 m, 2.70 m.

Test V60E2:

- mixture 60% oxyhydrogen and40% nitrogen;
- tube parameters:
  - wall thickness 6.02 mm;
  - tube length 5120 mm;
  - outer tube diameter 114.3 mm;
  - pressure transducer positions: 0.04 m, 4.99 m.

Only in this experiment a rupture of the tube was observed (see Figure 1). The authors of experiments have evaluated the possible position of DDT at 3,25 m, and position of rupture at 3.65 m.

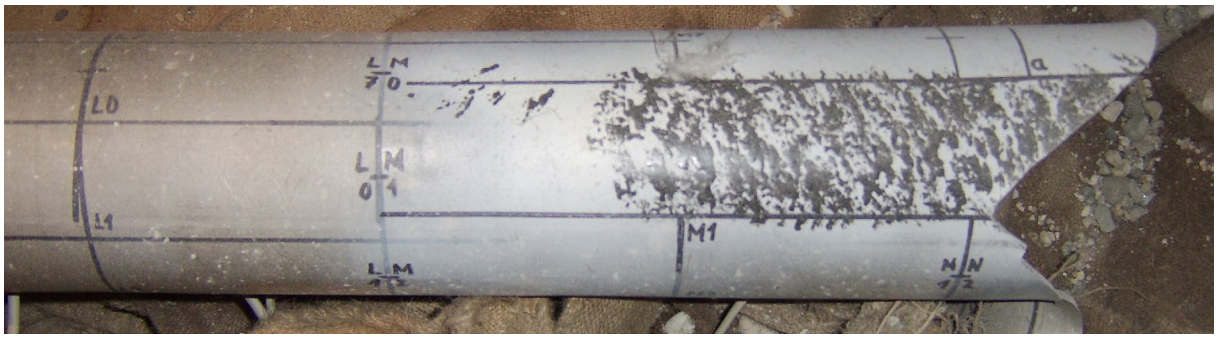

Figure 1. Breach of the tube in test V60E2.

3.0 DESCRIPTION OF THE MODEL

As in the previous implementation [4], the COM3D and ABAQUS two-way coupling provides exchange of data between these two codes on every time step and on the predefined set of nodes defined in both codes. From COM3D, the information on the 3D force acting at each node is transferred, and in the opposite direction from ABAQUS, the 3D displacement vector and 3D velocity vector are transferred. Additionally, from COM3D a heat flux associated with the node is transferred and the changed temperature of the wall is provided to COM3D.

In the new implementation the exchange nodes are associated with vertices of triangles forming a continuous surface that can change in shape in the course of simulation.

Note, the geometry model in both codes should be high degree consistent, especially in the areas where data transfer is performed.

3.1 Geometry model

For all simulations, the geometry models were fairly similar and had a rectangular computational area with a gas cylinder inside the area. The domain included additional space around the gas cylinder, which allowed the gas volume to expand. For the test V60E2, mesh resolution was 3.2 mm having 6.7 million cubic cells for the total calculation domain with internal gas volume of 1.3 million cells. For the test V100G2, the mesh size was 2 mm which resulted in 16.5 million cells for the calculation domain and 3 million cells for internal gas volume. For the test V80E3, the mesh size was 2.5 mm and 10 and 2 million cells for the total calculation domain and for gas volume respectively. The typical geometry overview is presented in Figure 2.

Figure 2. Geometry of test V60E2 simulation. A cut through the axis of the gas cylinder is shown.

The geometrical compound describing the internal surface of the tube is an aggregate of joined triangles forming a continuous cylindrical surface referred below as Joint Boundary Surface (JBS). The representative view of such JBS is presented in Figure 3.

The vertices of the JBS triangles were used as nodes for the exchange between COM3D and ABABQUS.

3.2 Governing equations

In the current work, the COM3D code solves a set of the Euler conservation equations for mass, momentum, energy and species.

$$(\rho)_t + (\rho u_i)_{x_i} = 0, \tag{1}$$

$$\left(\rho u_j\right)_t + \left(\rho u_i u_j\right)_{x_i} = \rho g_j - p_{x_j}, \quad (2)$$

$$(\rho e)_t + \left((\rho e + p)u_i\right)_{x_i} = \rho g_i u_i, \quad (3)$$

$$(\rho Y_\alpha)_t + (\rho Y_\alpha u_i)_{x_i} = \overline{\omega_\alpha}, \quad (4)$$

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

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

For ignition and flame propagation modeling, combustion model KYLCOM was used. Generally, KYLCOM model provides propagation of the flame with specified velocity, defined by one of turbulent flame velocity expressions available. In the current work, the burning speed was specified by the time-dependent formula targeted to provide the desired acceleration of the flame up to detonation.

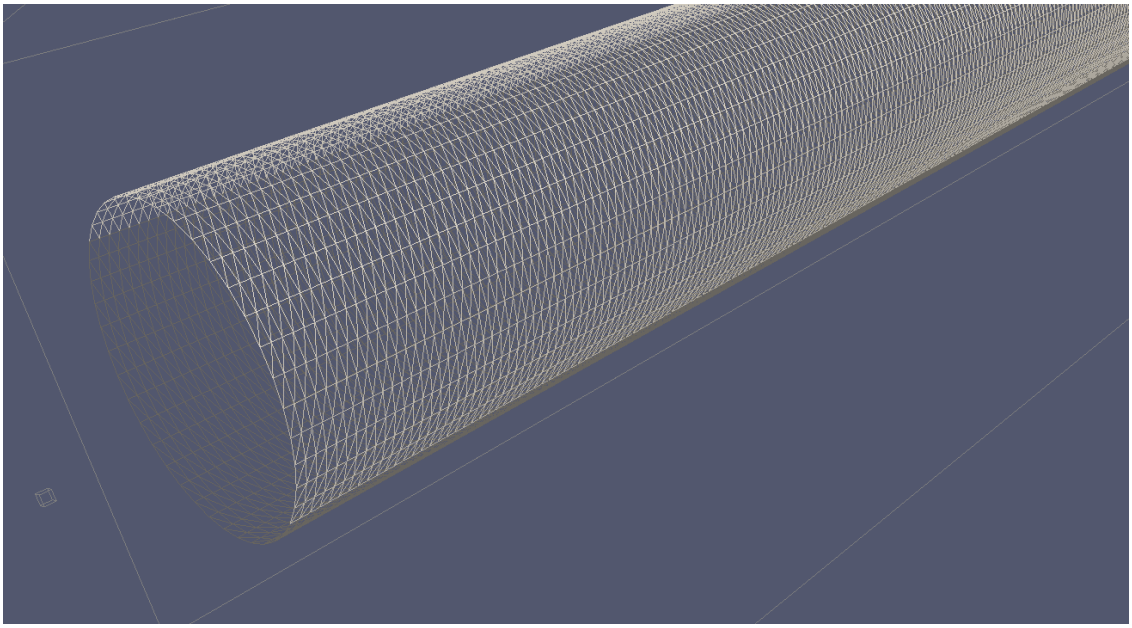

Figure 3. Joint boundary surface for test V60E2 test simulation.

3.3 Treatment of boundaries

For the accounting of exact boundary position which does not coincide with the faces of the rectangular mesh, the concept of the partial blocking of the mesh cell was implemented. The idea consists in the accounting of only that part of the mesh cell which actually belongs to the gas volume. The gas fluxes transported through the faces of the cubic cell are also proportional to the parts of each face which are open to the adjacent cells. The gas-dynamic equations are modified accordingly.

Numerically, the procedure consists in the calculation of the intersection of the JBS and the mesh cube of each cell at the boundary. For the higher accuracy and simplification of the interpretation, calculation of the cube intersection was split to the calculation of six tetrahedrons' intersections.

In Figure 4, the tetrahedrons constituting mesh cube are presented. For each tetrahedron, intersections of edges, e.g., e0, e3, e8, e12, e13, e14 for tetrahedron #1, are calculated and then partial volume blockage and face blockage are exactly computed.

For the characterization of the intersection, the notion of Volume Blockage Ratio (VBR) defining which part of the cell is beyond the gas volume, and Face Blockage Ratio (FBR) defining which part of the cell face is outside of the gas volume, were introduced.

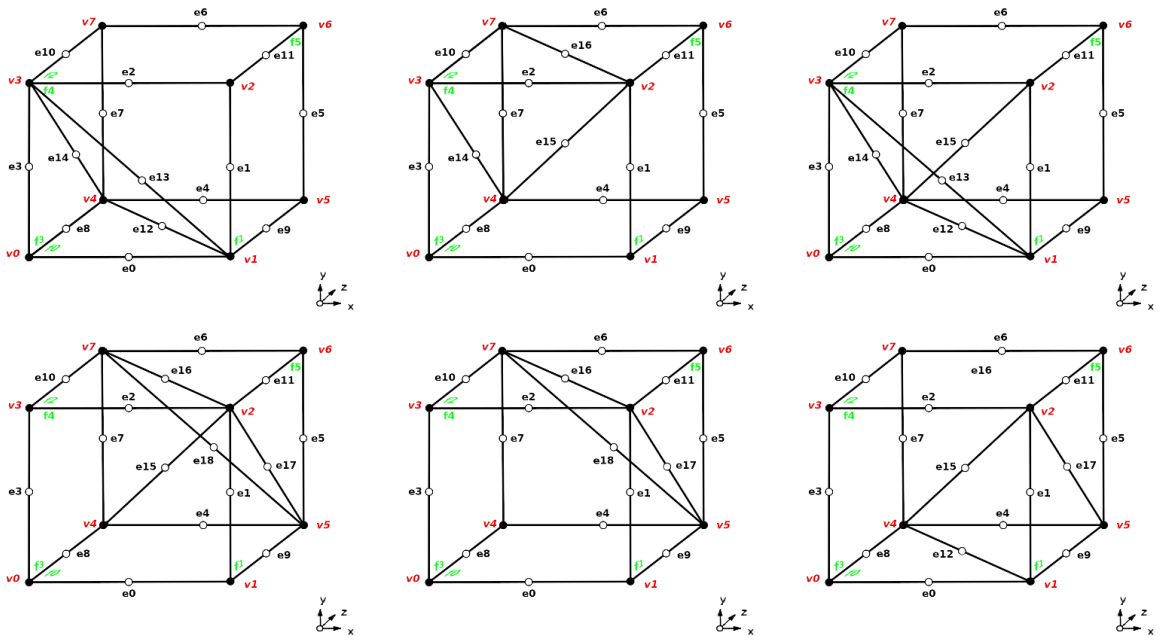

Figure 4. Tetrahedrons constituting mesh cell cube.

Evaluation of the cell blockage is performed on each time step after obtaining spatial data from ABAQUS. This provides equivalent movement of the boundary and corresponding changes of the gas-dynamics. First, for each cell intersections of the 6 cell edges with the updated surface triangles are calculated:

- In case of no intersections, VBR is assigned equal to 0 or 1 for gas or solid correspondingly;
- For discovered external edge intersections, detailed sub-cell structure is calculated. For six internal tetrahedrons VBR and FBRs are calculated assuming that all intersections of the tetrahedron edges belong to one plane. Such assumption disregards cases when vertices or edges of the interface surface are located inside the tetrahedron. This assumption reduces accuracy of the evaluation, while making the algorithm stable and distinct.

This algorithm allows the effective cell volume to be changed during simulation depending on the force applied to the cell boundary and the material of the cell, when the physical (real) boundary moves inside the cell, i.e., a cell can be partially filled with gas and partially with solid.

When a crossing surface leaves a cell, the calculating mesh is re-generated, otherwise accounting of the wall dislocation is performed using the sub-grid described model. The model includes control of the

evaluated cell fraction occupied by gas/solid material, and corresponding correction of fluxes through the cell boundaries and field parameters inside the cell.

So, at each time step, COM3D gets a new set of blocking ratios for cells and faces. These blocking ratios are used to correct fluxes of important cell properties (mass, energy, momentum, species).

The following issues need to be considered when applying modified blocking factors:

1. Conservativity. Without blocking, the total amount of, say, mass is equal to density times cell volume, which is constant. This value should now be corrected by a factor (1-VBR). Thus, if the blocking ratio is changed, we need to multiply the average number of cells by the factor $(1\text{-}VBR_{old})/(1\text{-}VBR_{new})$.

2. Deleted cells. If the boundary moves in such a way that at the next time step the cell becomes completely blocked, then in subsequent calculations it will be considered solid. In this case, we need to redistribute mass, energy, momentum, etc. from this cell to some neighboring cells. We are currently using the cell that has the smallest blocked face with the cell in question at the previous time step. You can think of this operation as if we were merging two cells, calculating the total in that cell relative to the total old unlocked volume, and then allocating that value to the new unlocked volume.

3. New cells. In a way as described in the previous paragraph, the border can move to a cell that was previously completely blocked. Now this cell should be considered as a gas cell and we need to assign some values to this cell. As in the previous case, we are looking for a cell with the least blocked edge (new blocking). We then take the values from that cell and spread across two cells in proportion to the unlocked volume in those two cells.

4. Small cells. In some cells, the blocking factor can be close to 1. This means that the effective time step is determined not by the cell size, but by some fraction of it (in the worst case, dx*(1-VBR)). This fact can affect the stability of the numerical scheme. To solve this problem, we merge this cell with the adjacent cell (the cell with the least blocked face). As in the previous paragraphs, we find the total value of the stored quantities in these two cells in relation to the unlocked volume and distribute back proportionally to unblocked volume. After such a procedure, the densities of energy, momentum, etc. in these two cells will be the same. From the point of view of the numerical scheme stability, these two cells can now be considered as one large cell. This averaging procedure happens not only when new blockage is known, but also on every internal sub-step of the calculation procedure.

4.0 SIMULATIONS AND RESULTS

Since in all the experiments considered the exact position of the DDT was not known, and the pressure records were known only for a few positions or were not available at all, the position of the DDT was adjusted in the simulation in such a way as to obtain the best reproduction of the residual stretching.

The combustion process was modeled using the KYLCOM model with prescribed burning speed in the initial phase and after reaching DDT parameters, detonation model was used. The very reactive mixtures and high initial pressure in the experiments does produce products with relatively high content of hydrogen and numerous compounds of O, H, and N. For example, mixture used in V80E3 of 80% oxyhydrogen and 20% nitrogen, products can include 8% of unreacted hydrogen. To avoid utilization of the detailed reaction scheme, the equivalent one-step reaction was used with products corresponding to the equilibrium state. The equilibrium state was calculated using CANTERA [5].

While all of the calculations were performed using the three-dimensional COM3D code, several simulations were performed for comparison using the one-dimensional COM1D code. The results are quite similar, which indicates a high axisymmetry of the simulated process. The simulation result convergence was proved using different resolutions of COM3D mesh and of vertex density of JBS.

For the material properties in ABAQUS, the properties of the austenitic steel (in SI units), as they are in ABAQUS input (for more details, see [7]):

- Conductivity 15.,
- Density 7800.,
- Elastic 1.75e+11, 0.3
- Inelastic Heat Fraction 0.9,
- Plastic, hardening=JOHNSON COOK: 2.40e8,1.220e9, 0.66, 0.77,1809., 298.
- Rate Dependent, type=JOHNSON COOK: 0.0198,1.
- Specific Heat 500.,

4.1 Test V80E3

For this experiment, only data on the residual stretch of the tube were available, therefore when reproducing it, we were forced to focus only on the available data. In the calculations, in order to avoid complications connected with the complex structure of the combustion wave taking place in the experiment, the spherical ignition source was replaced by a flat sheet, which initiates a quasi-one-dimensional flow.

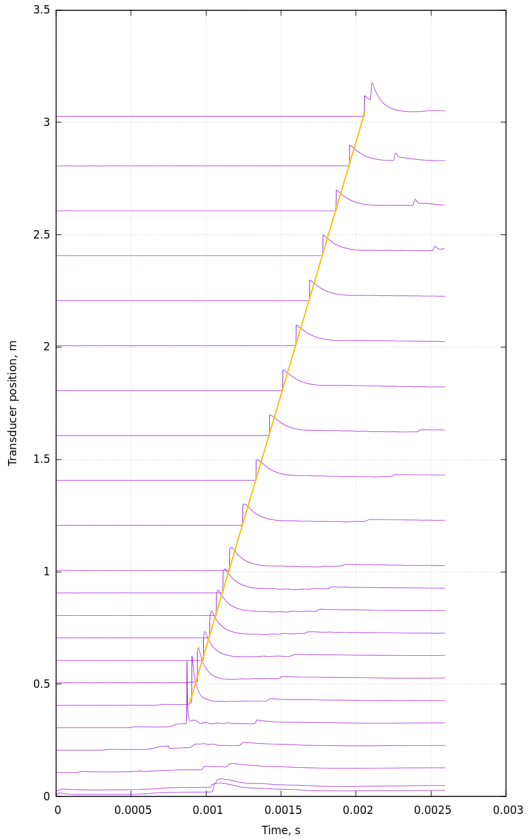

Figure 5. X-t diagram of overall process for simulation of V80E3 test. Yellow line shows the trajectory of the detonation wave with the shock speed of 2824 m/s.

To obtain a residual stretch corresponding to that observed in the experiment, it was found that the location of the DDT event should be at a distance of 0.35 m from the ignition. The initial combustion phase was simulated using standard COM3D combustion model KYLCOM with the prescribed flame acceleration law, and at 0.95 ms the model was switched to detonation one. After detonation onset, on a distance ≈ 0.2 m, the detonation speed reduced to the values close to the steady state values of 2824 m/s (see Figure 5). Note, that theoretical Chapman-Jouguet prediction gives detonation speed for this mixture equal to 2639 m/s. This discrepancy could be connected with the difference in evaluation of the thermodynamic equilibrium of the equivalent reaction products in the COM3D and CANTERA program.

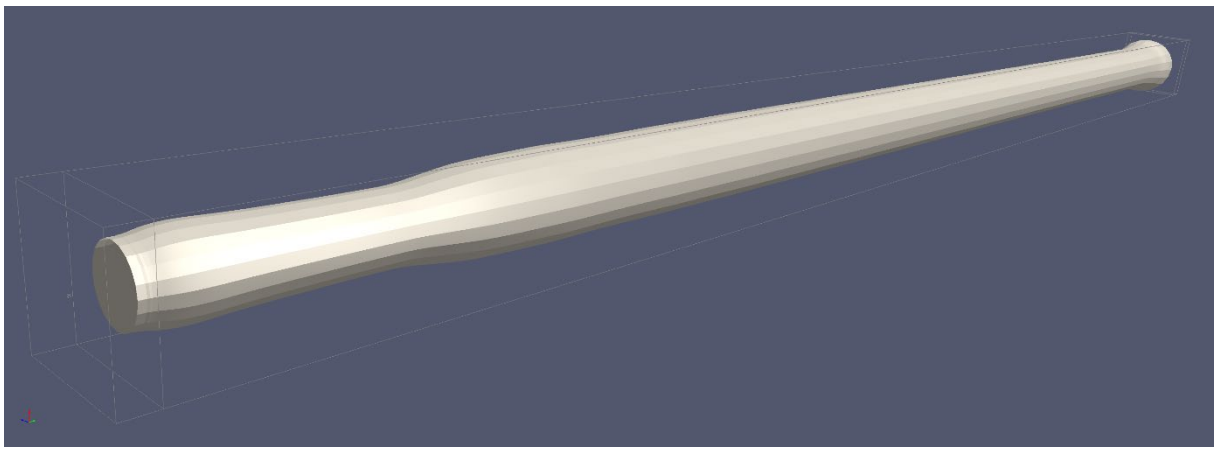

Figure 6. JBS at 2.53 ms after ignition.

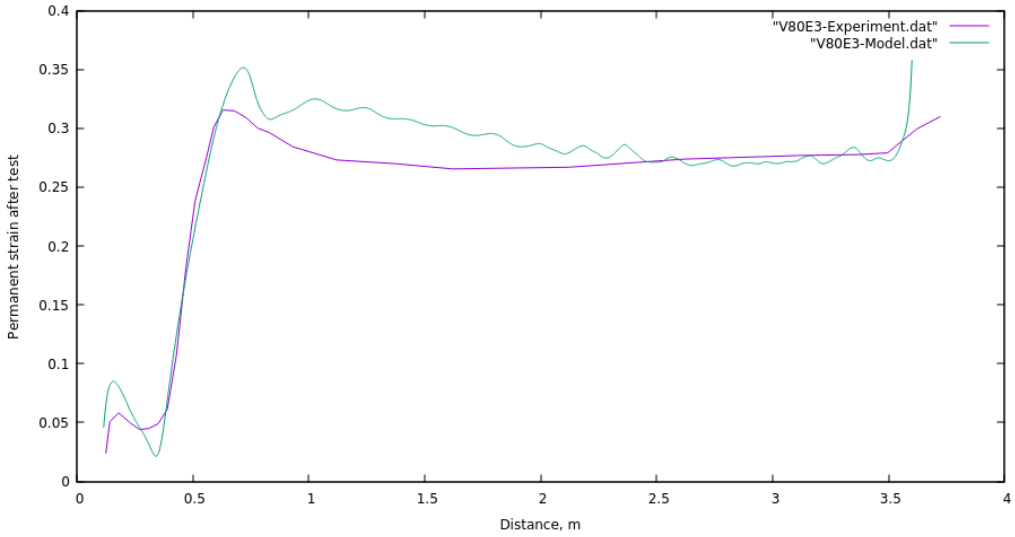

Figure 7. Comparison of the residual stretch in the experiment and in the simulation.

Comparison of the measured in the experiment and the calculated residual stretch demonstrates that main characteristics of the process are reproduced reasonably well. The excessive stretch at the end of the tube is definitely connected with simplified boundary conditions, which assume fixed position of the tube ends, preventing the tube to elongate in axial direction. It should also be taken into account that in the experiment the far end of the pipe was equipped with a rupture membrane, which excluded the appearance of a reflected wave propagating backward along the pipe. The excessive stretch in the region

downstream the DDT position can be connected again with the restriction of the tube elongation and presence of the reflected wave or with the not fully adequate detonation relaxation from DDT to steady state parameters, as discussed above.

4.2 Test V100G2

In contrast to the experiment V80E3, in this experiment the mixture was more reactive, namely it was pure oxyhydrogen. As it can be expected, the DDT process took place at an earlier stage and at a shorter distance from ignition position. For this experiment, data on the propagation of pressure wave were available, which made it possible to verify the parameters of the ongoing process.

In this test, to produce residual stretch corresponding to the experimental, the DDT location was found to be 0.115 m from ignition. The numerical procedure consisted also from consecutive utilization of KYLCOM model with the prescribed flame acceleration law and detonation model after 0.38 ms.

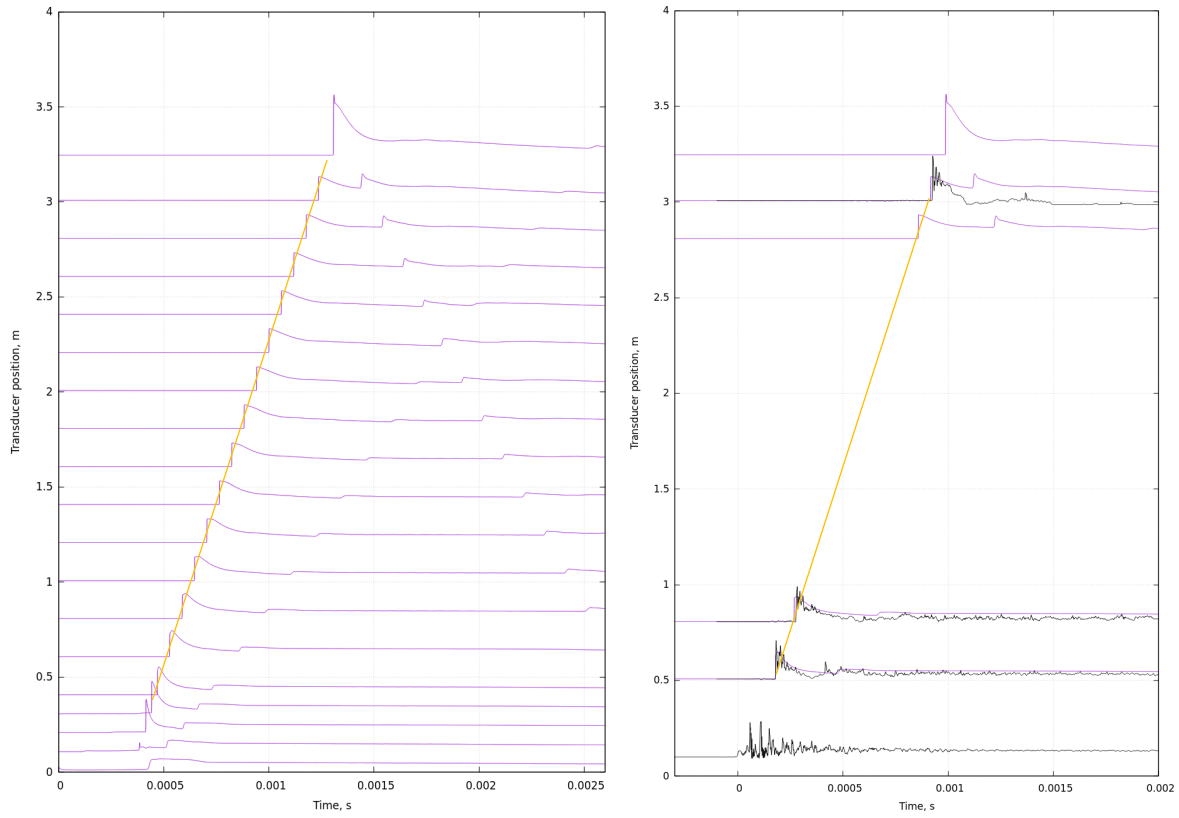

Figure 8. X-t diagram of overall process for V100G2 test. Left: simulation with DDT at 0.115 m from ignition position. Right: Comparison of experimental records with corresponding numerical transducers. Yellow line shows the trajectory of shock waves.

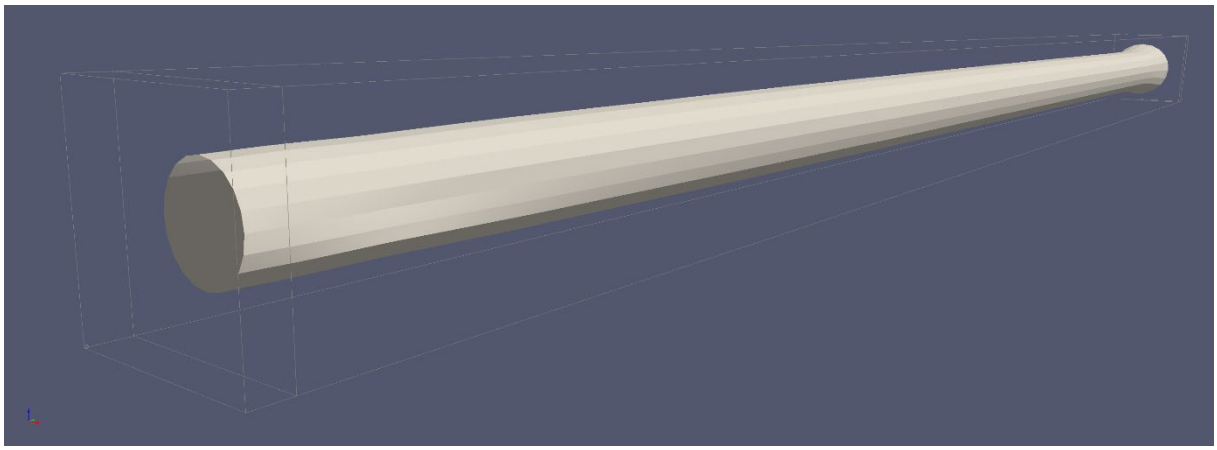

Figure 9. JBS at 2.6 ms after ignition.

Note, that comparison of the experimental and calculated pressure records was not always straightforward, since positions of the pressure transducers were not always definitely specified. Among possible (2.79 m - 3.136 m) indicated locations, the position close to 3 m best matches the steady state detonation parameters, with detonation speed in this case is 3356 m/s.

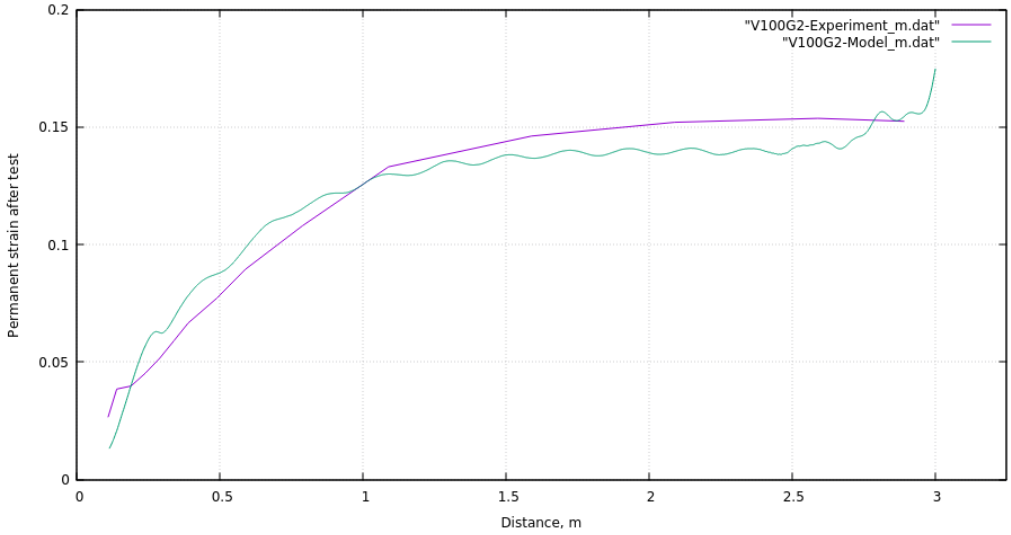

Figure 10. Comparison of the residual stretch in the experiment and in the simulation.

As in the previous test, comparison of the experimental and calculated residual stretch demonstrates quite satisfactory agreement. The excessive stretch at the end of the tube and in the region of the detonation wave relaxation immediately after DDT, can also have the same origins as in the previous test.

4.3 Test V60E3

In this test, the least reactive mixture, namely 60% oxyhydrogen + 40% nitrogen, was used, however only in this experiment a rupture of the tube was observed. The rupture position was between 3 m and 4 m from the ignition position. Pressure records were available only near both ends of the tube, showing strong detonation wave at far end and weak pressure wave at position close to ignition.

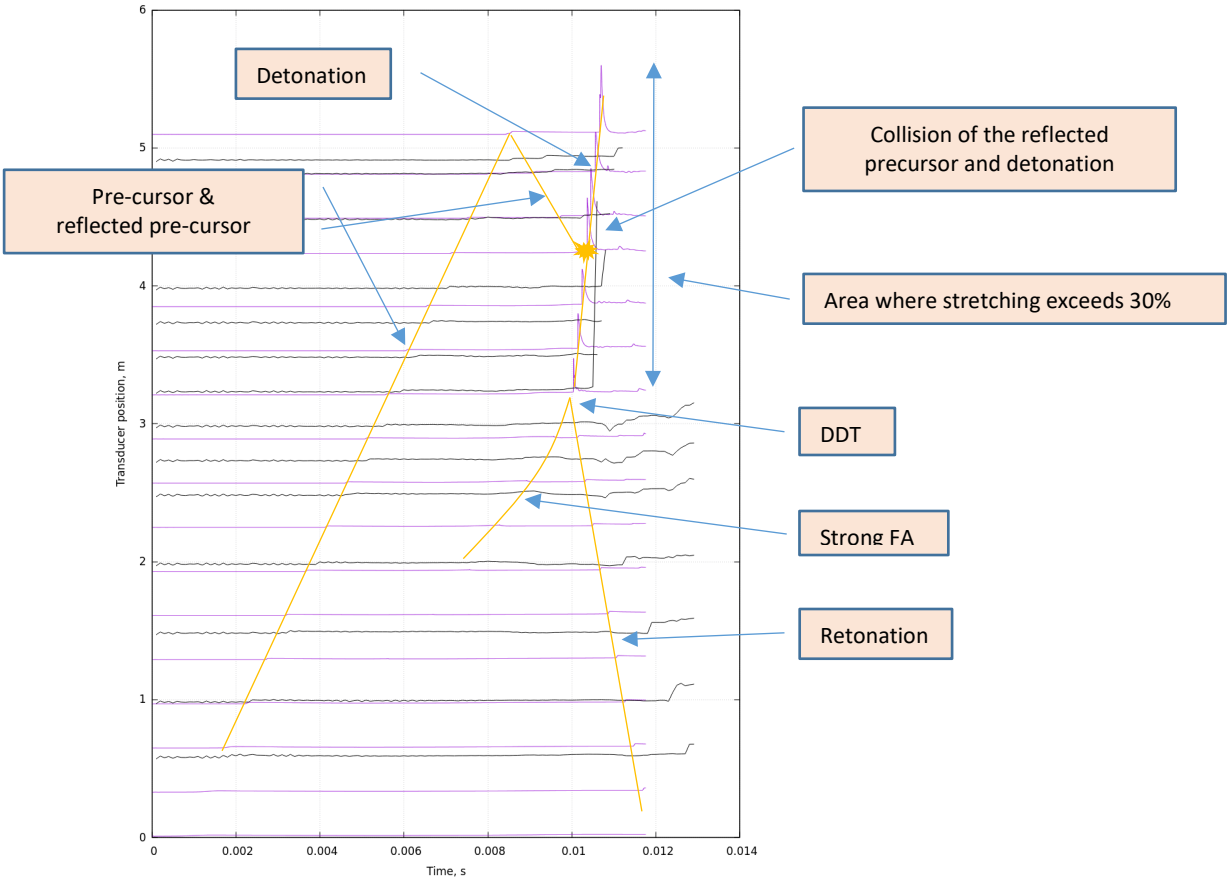

Figure 11. X-t diagram of the whole process for conditions of V60E3 test.

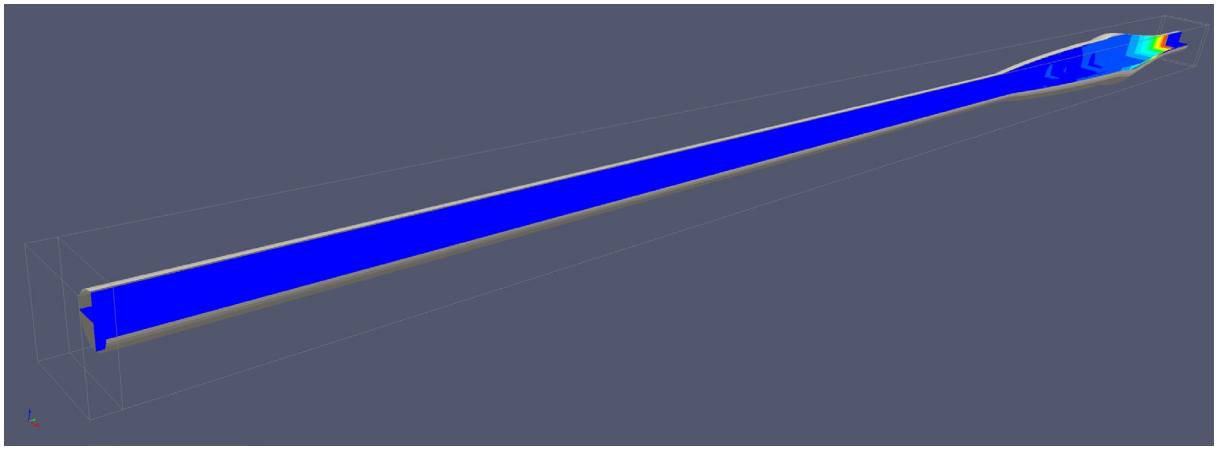

Figure 12. Pressure field and JBS at 10.6 ms after ignition. Red color corresponds to $2.78 \cdot 10^8$ Pa.

In simulation, the flame acceleration dependency was selected to produce DDT at position of 3 m. However, the strongest stretching was observed at a position about 1 m downstream. The analysis of the X-t diagram shows that at this position the detonation wave meets the precursor pressure wave reflected from the far end. At this moment the detonation wave undergoes considerable amplification reaching more than 3500 bar. Note, that the maximum stretching (see Figure 12) is located at position 4.2 m from ignition.

Due to the material properties in ABAQUS, the local breach of the tube walls in calculation was not simulated, however the observed stretching was considerably higher than in other tests, and for the real material would definitely lead to the tube rupture.

Thus, we can conclude that the possible pipe rupture in these experiments can be unambiguously associated with the phenomenon of detonation wave amplification when detonation passes into a pre-compressed medium, as in the case of a collision with a reflected precursor wave. The DDT process without additional intensification does not lead to the tube destruction even in case of considerable deformations.

5.0 CONCLUSION

New model of boundary conditions describing exact 3D shape of the confining surface applied on equidistant mesh was developed, successfully implemented and tested. The model allows realize a real-time data exchange with finite-element code ABAQUS - © Dassault Systèmes.

New capabilities to perform simulations with exact 3D variable geometrical environment using high quality finite-element analysis by ABAQUS and gas-dynamic data from COM3D provide possibility to perform coupled gas-dynamic and material stress analysis.

Using the new model, three simulations based on the experimental data were carried out and demonstrated the necessity of the coupled approach. The obtained numerical results demonstrate good agreement with the available experimental data.

The coupled approach can be considered as a new safety analysis tool that is targeted to identify potentially hazardous locations or components in appliances.

6.0 REFERENCES

[1] E. Studer, S. Koudriakov, B. Cariteau and R. Scarpa, "Detailed examination of deformations induced byinternal hydrogen explosions : Part 2 Experiments.," in *ICHS 2019 - International Conference on HydrogenSafety*, Adelaide, 019.

[2] A. Kotchourko, A. Lelyakin, J. Yanez and G. Halmer, *COM3D: Turbulent Combustion Code User's Guides,* 2021.

[3] S. Offermanns and W. Stadtmüller, "Untersuchungen zur Analyse von Radiolysegasdetonationen im Hinblick auf Nachrüstungen und zukünftige Auslegungen von Rohrleitungen : Abschlussbericht, Investigations of detonations due to radiolysis gas in terms of retrofitting and future design of piping," Materialprüfungsanstalt, Universität Stuttgart;, Stuttgart, 2015.

[4] S. Ofermanns, E. Ross and W. Stadtmüller, "Structural Response of Thin-walled Austenitic Pipes to Internal Gaseous Detonation Loading," in *Proc. ASME IMECE 2011, IMECE2011-63352*, Denver, USA, 2011.

[5] A. Kotchourko, A. Lelyakin and T. Jordan, "Modeling of hydrogen flame dynamics in narrow gapwith bendable walls," in *7th International Conference on Hydrogen Safety (ICHS 2017)*, Hamburg, 2017.

[6] D. G. Goodwin, R. L. Speth, H. K. Moffat and B. W. Weber, *Cantera: An Object-oriented Software Toolkit for Chemical Kinetics, Thermodynamics, and Transport Processes,* 2021.

[7] S. Offermanns and S. Weihe, "Damage and Failure of Thin-Walled Piping under Detonative Loading" in: 13th International Conference on Mechanical Behaviour of Materials," in *ICM-13*, Melbourne, Australia, 2019.