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Modeling of Tube Deformation and Failure under Conditions of Hydrogen Detonation

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Motivation

- 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.

Experiments

- 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.*
    - *No pressure transducers*
- 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.*

- Three experiments on the study of austenitic tube behavior under pressure load:
  KIT/ProScience GmbH
  MPA/Stuttgart University
- The tubes were equipped with pressure and displacement transducers.
- Mixture of 2 H_2 : 1 O_2 (oxyhydrogen) diluted with nitrogen;
  initial P = 70 bar,
  T = 298.15 K.
  Rupture membrane at far end.

Experiment

- Test V60E2:
  - mixture 60% oxyhydrogen and 40% 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 one test was with tube rupture

The authors of experiments have evaluated the - possible position of DDT at 3,25 m
- and position of rupture at 3.65 m

Numerical model description

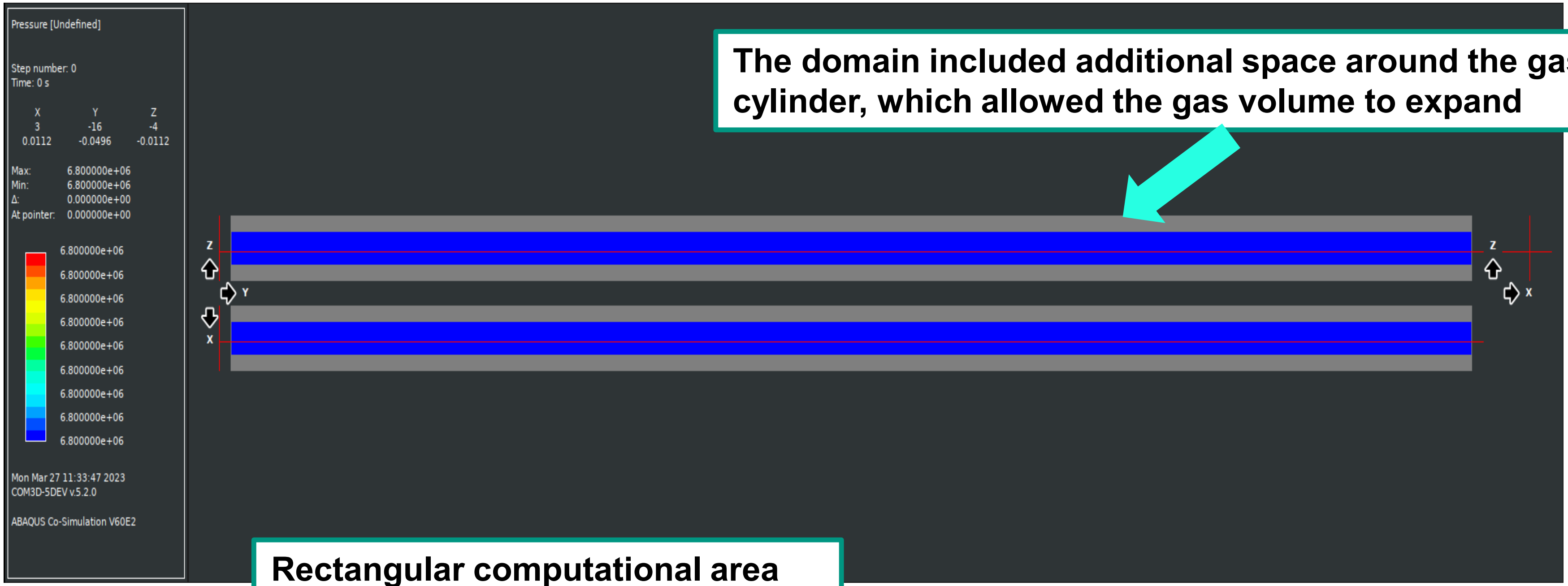
- Euler set of gasdynamic equations
  - $(\rho)_t + (\rho u_i)_{x_i} = 0,$
  - $\left(\rho u_j\right)_t + \left(\rho u_i u_j\right)_{x_i} = \rho g_j - p_{x_j},$
  - $(\rho e)_t + \left((\rho e + p)u_i\right)_{x_i} = \rho g_i u_i,$
  - $(\rho Y_\alpha)_t + (\rho Y_\alpha u_i)_{x_i} = \overline{\omega_\alpha},$
  - $e = \sum_{\alpha=1}^{N} \frac{Y_\alpha}{\mu_\alpha}(h_\alpha + \Delta h_\alpha^0 - RT) + \frac{1}{2} u_i u_i \;,$
  - $Y_\alpha = \frac{\rho_\alpha}{\rho},$
  - $\overline{\omega_\alpha}$ - KYLCOM combustion model

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 flame acceleration up to detonation.

Geometry model

- V60E2: mesh resolution 3.2 mm with 6.7 Mcell total / 1.3 Mcell gas
- V100G2: mesh size 2 mm with 16.5 Mcells total / 3 Mcell gas
- V80E3: mesh size 2.5 mm with 10 Mcells total / 2 Mcell gas



Pressure [Undefined]

Step number: 0
Time: 0 s

X	Y	Z
3	-16	-4
0.0112	-0.0496	-0.0112

Max: 6.800000e+06
Min: 6.800000e+06
Δ: 0.000000e+00
At pointer: 0.000000e+00

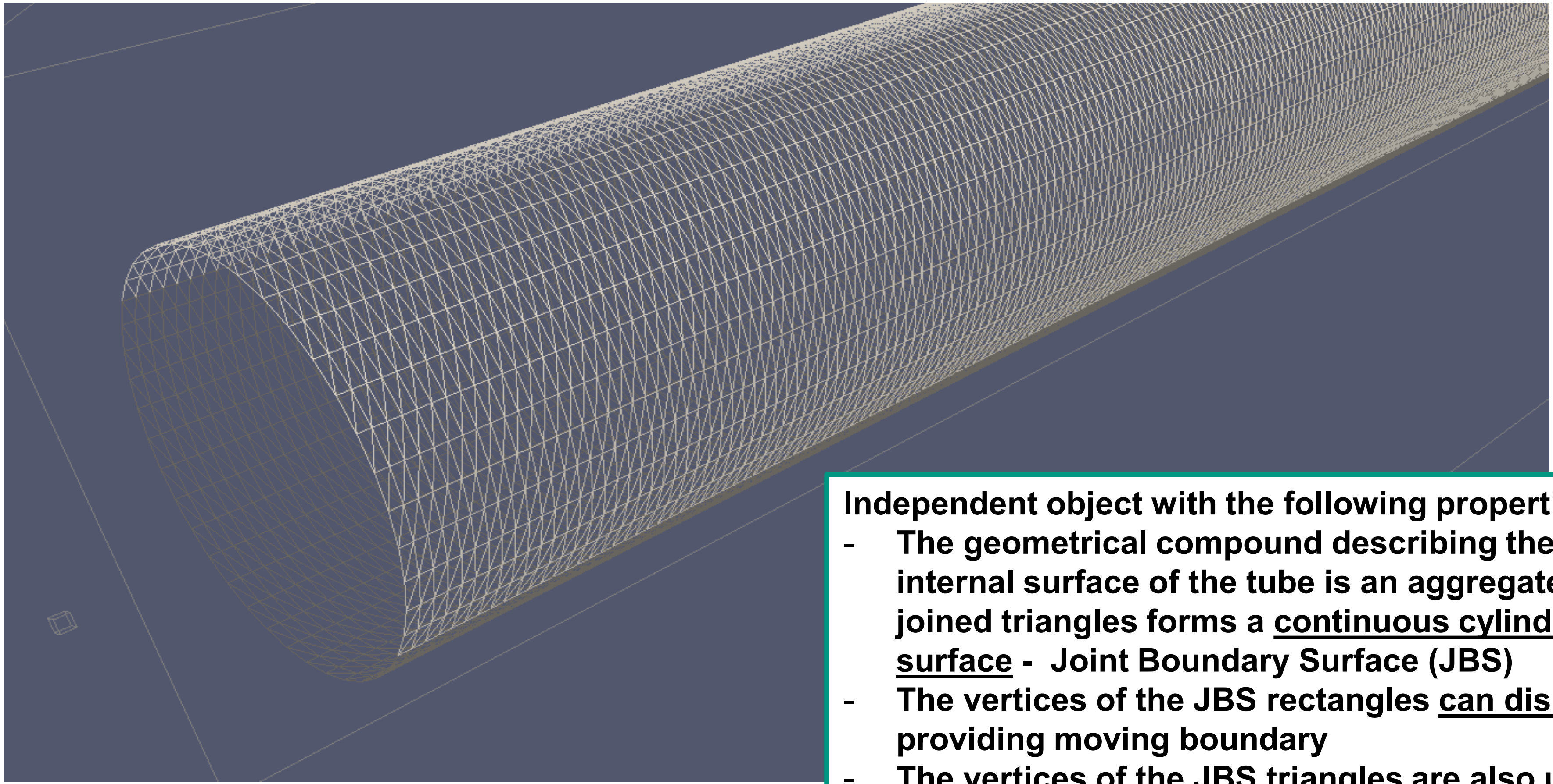
Mon Mar 27 11:33:47 2023
COM3D-5DEV v.5.2.0

ABAQUS Co-Simulation V60E2

The domain included additional space around the gas cylinder, which allowed the gas volume to expand

Rectangular computational area with a gas cylinder inside the area

Geometry model for boundary



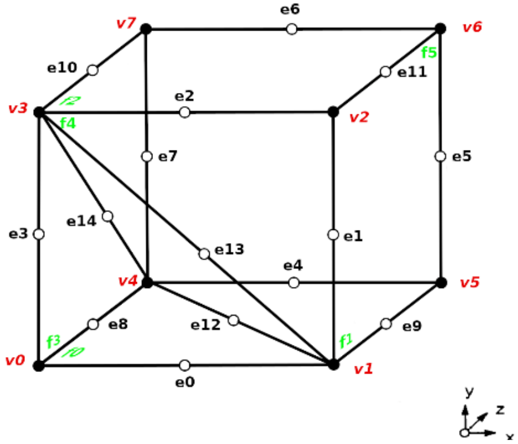
Independent object with the following properties:

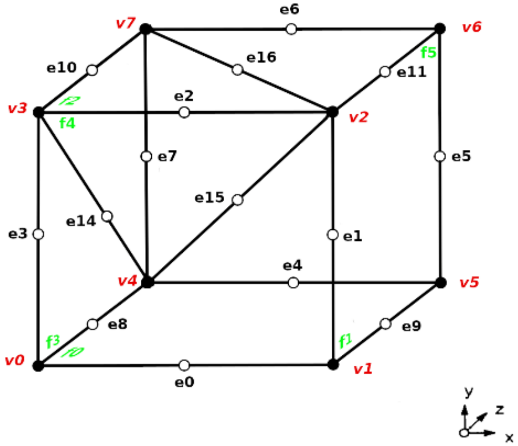
- **The geometrical compound describing the internal surface of the tube is an aggregate of joined triangles forms a <u>continuous cylindrical surface</u> - Joint Boundary Surface (JBS)**
- **The vertices of the JBS rectangles <u>can displace</u> providing moving boundary**
- **The vertices of the JBS triangles are also used as nodes for the <u>exchange</u> between COM3D and ABABQUS (forces and heat fluxes)**

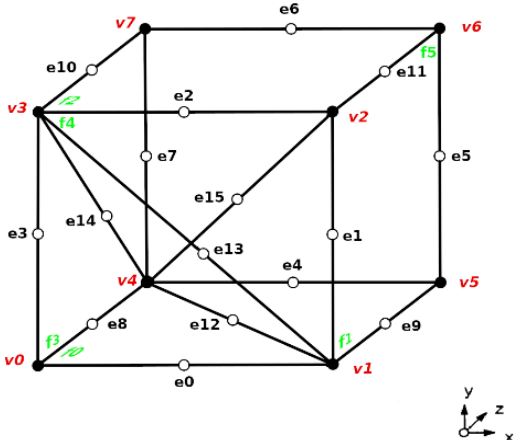
Boundary treatment

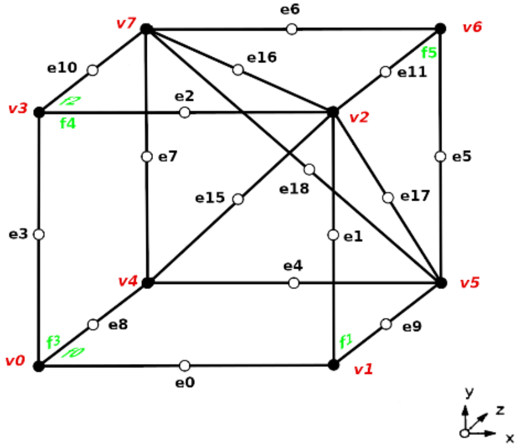
- The concept of the partial blocking of the mesh cell was implemented
- Idea: accounting only that part of the mesh cell which actually belongs to the gas volume
  - Mesh volume is gas volume
  - Gas fluxes through the mesh faces ~ face parts open to the adjacent cells
  - Gas-dynamic equations are modified accordingly
- When Joint Boundary Surface (JBS) moves, it can arbitrarily intersect the faces of the rectangular mesh
- Numerically, the procedure consists in the calculation of the intersections of the JBS and the mesh cube for 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

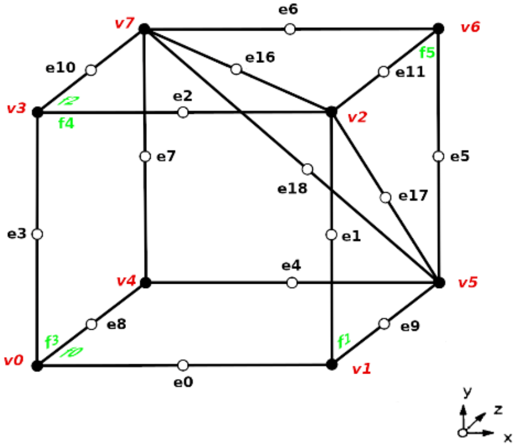
Boundary treatment

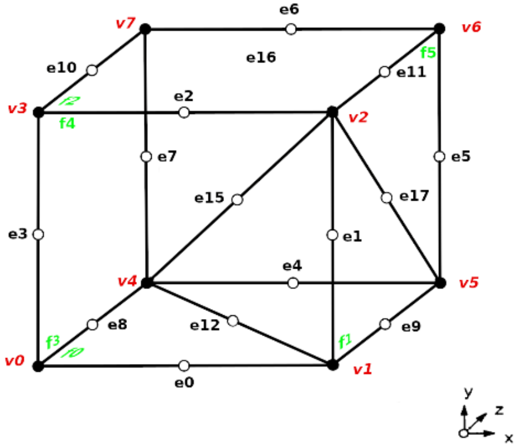












Life cycle of a mesh cell

- The following issues need to be considered when applying modified blocking factors:
  - *Conservativity*. With the changing of cell blocking the conserving values, as e.g., density should be corrected by a factor (1-VBR_{old})/(1-VBR_{new}).
  - *Cell death*. When a cell submerges into the wall, the mass, energy, momentum, etc. should be distributed over neighboring cells. Currently, the values are forwarded to the cell with the smallest blocked face.
  - *Cell birth*. When a cell emerges from the wall, its content is taken again from the cell with smallest blocking in proportion to the unlocked volumes.
  - *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, Δx*(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 for deleted/inserted cell, first the total values of the stored quantities in these two cells are calculated and then after the step thay are distributed back proportionally to unblocked volumes.

Simulation details

- Experimental exact position of the DDT was not known (pressure records only for few positions) - the position of the DDT in simulations was adjusted to obtain the best reproduction of the residual stretching
- Combustion process was modeled using the KYLCOM model with prescribed burning speed initially + detonation after DDT model
- Typically used mixtures do produce products with high content of hydrogen and numerous compounds of O, H, and N, e. g., in V80E3 (80% $2H_2:O_2$ + 20% N_2), products can include 8% of unreacted hydrogen.
- The equivalent one-step reaction was used with products corresponding to the equilibrium state by CANTERA.
- For the material properties in ABAQUS, the properties of the austenitic steel (in SI units), as they are in ABAQUS input :
  - 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.,

Simulation of test V80E3

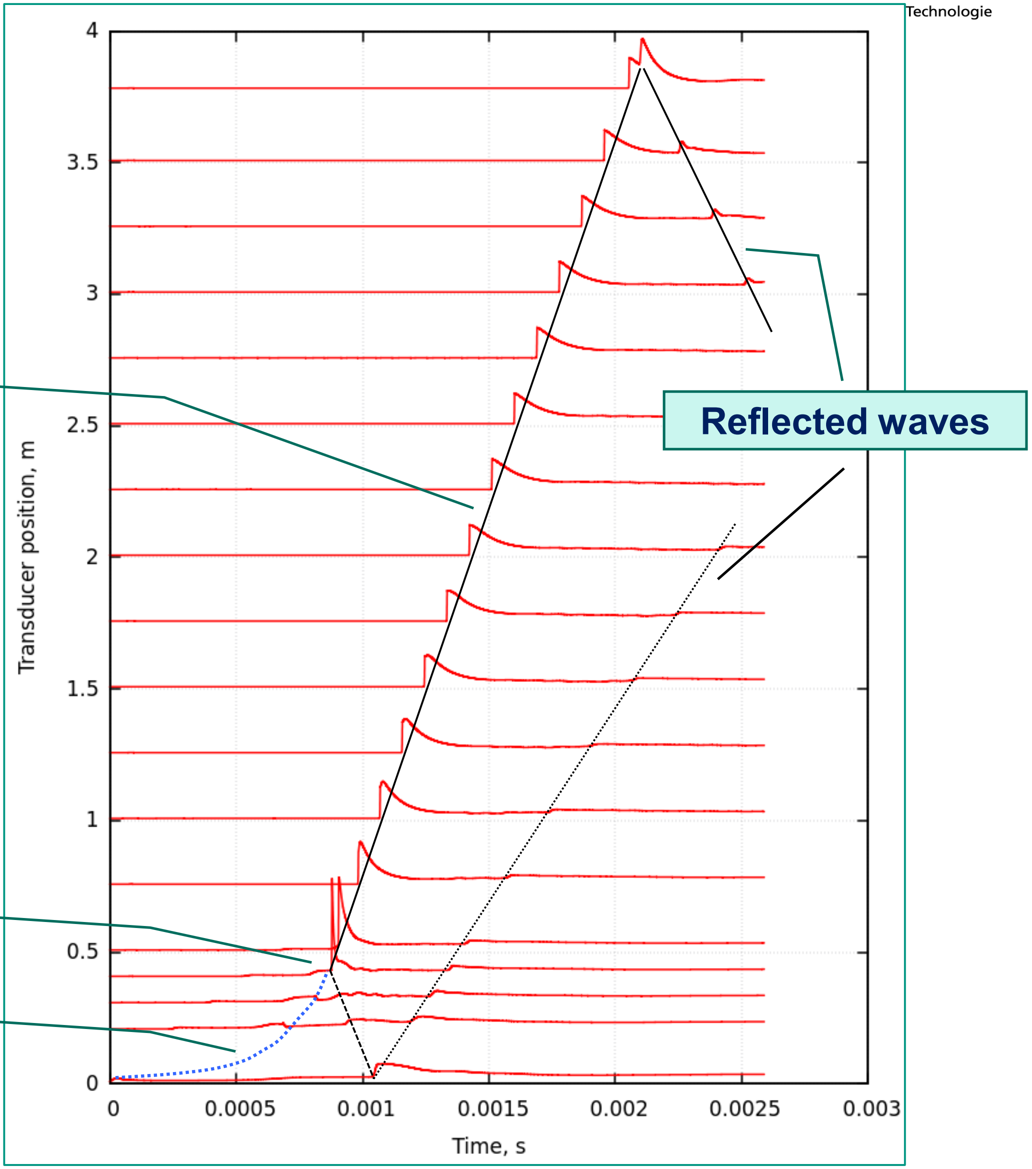
80% oxyhydrogen + 20% nitrogen

Average detonation speed 2824 m/s

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 vs theoretical Chapman-Jouguet prediction of 2639 m/s

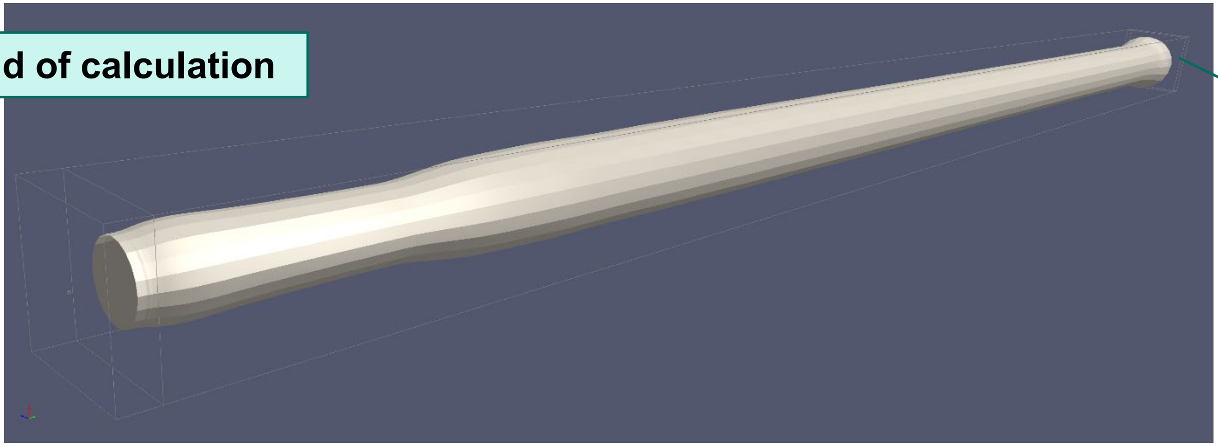
DDT

Flame acceleration phase

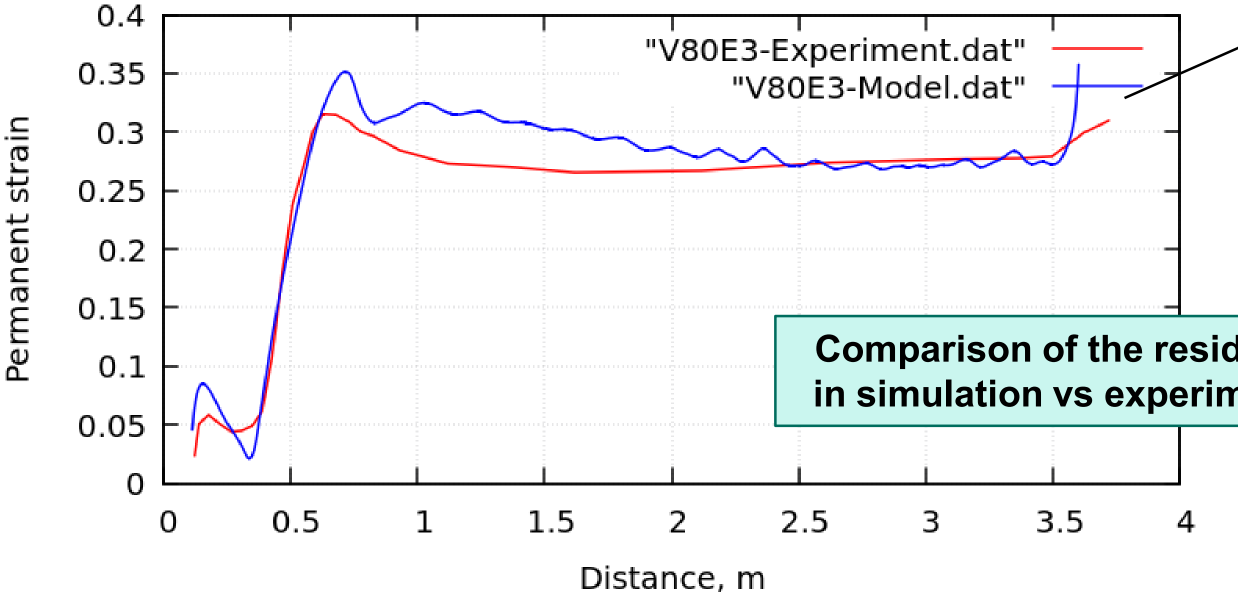


Residual deformation

JBS at the end of calculation



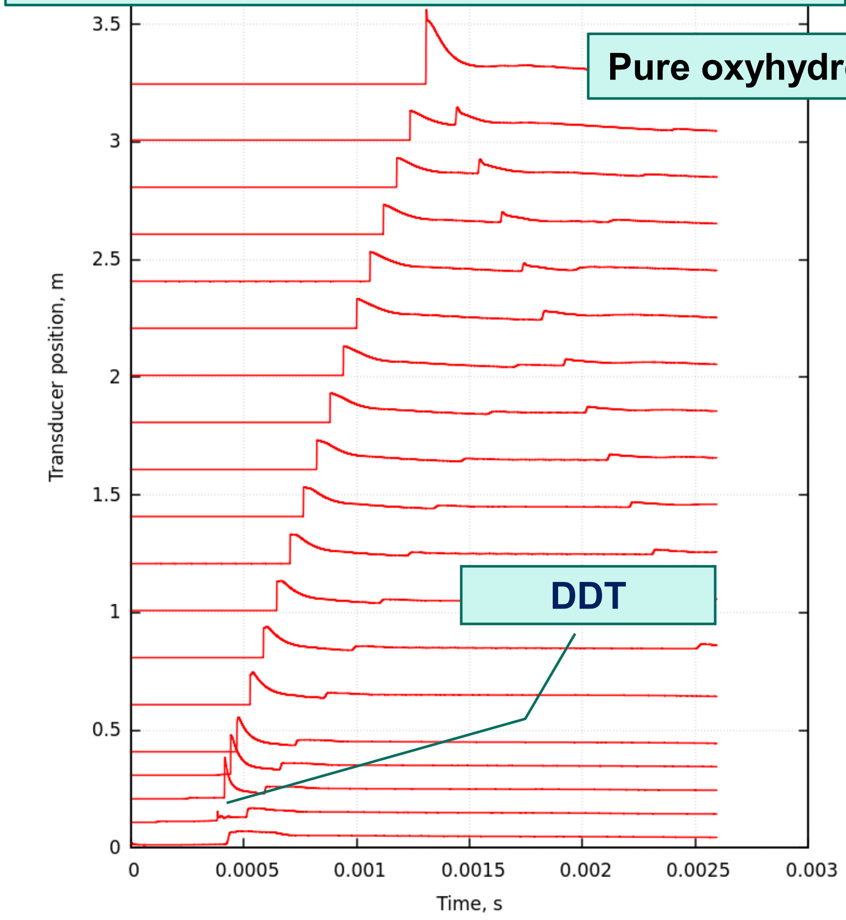
Excessive deformation



Comparison of the residual strain in simulation vs experimental data

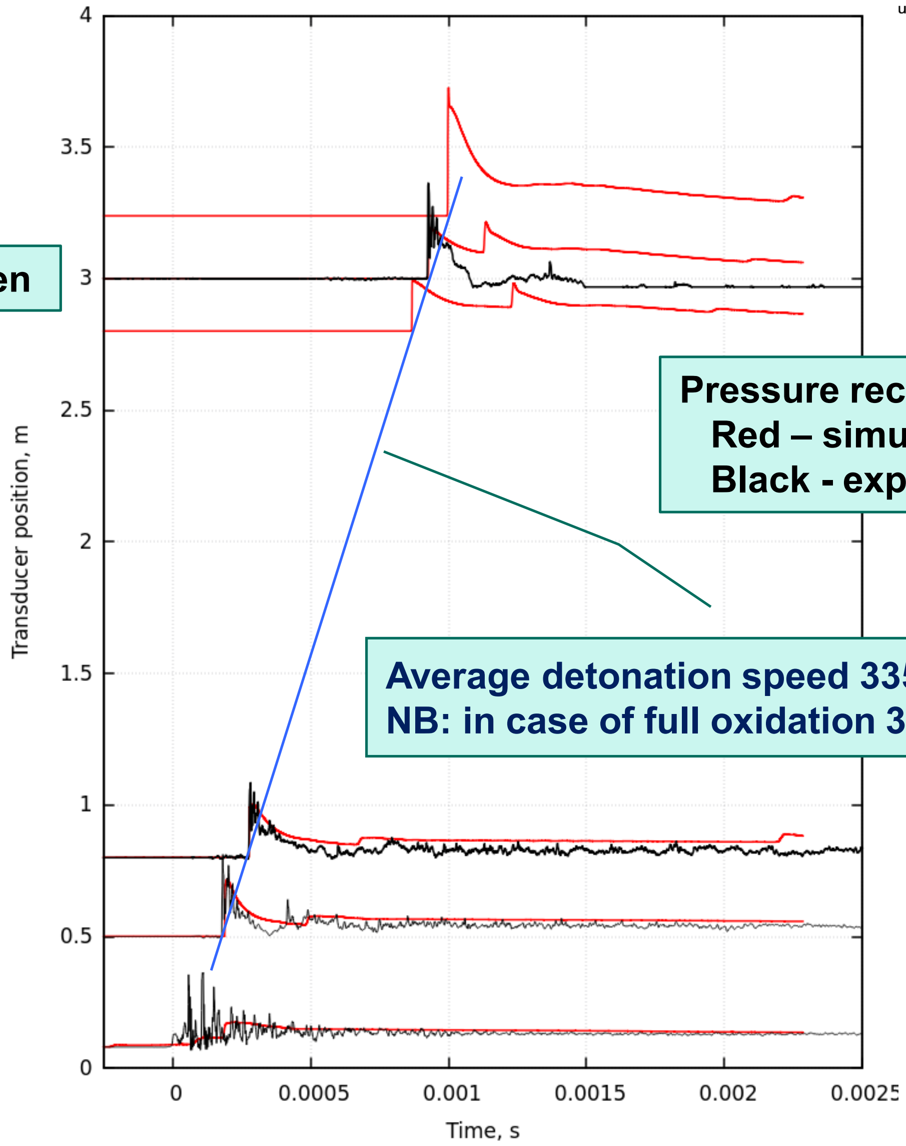
Simulation of test V100G2

The DDT location was found to be at 0.115 m to produce residual strain corresponding to that observed in the experiment



Pure oxyhydrogen

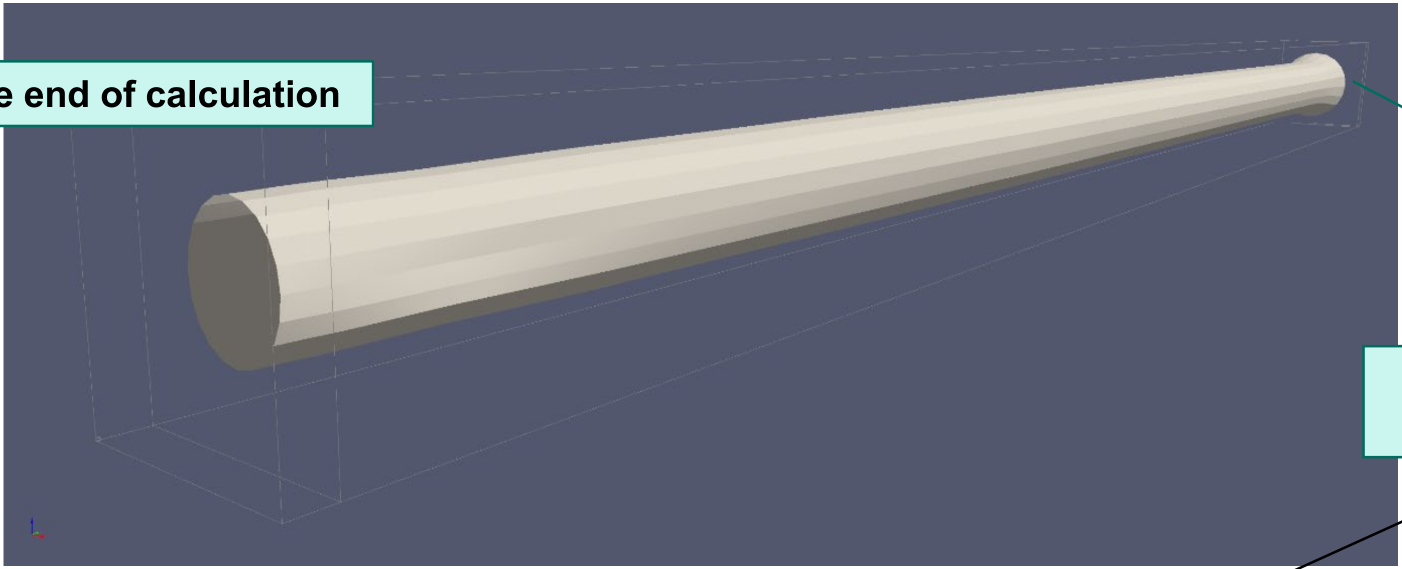
DDT



Pressure records:
Red – simulation
Black - experiment

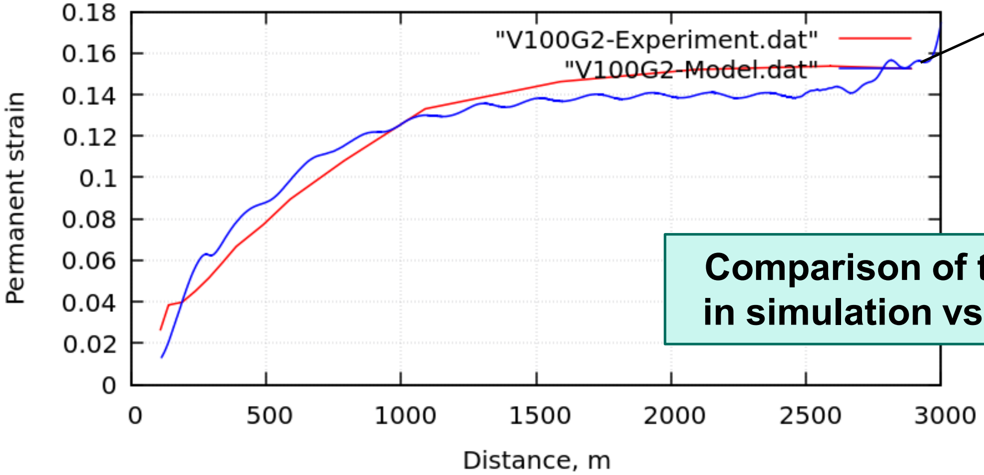
Average detonation speed 3356 m/s
NB: in case of full oxidation 3480 m/s

Residual deformation



JBS at the end of calculation

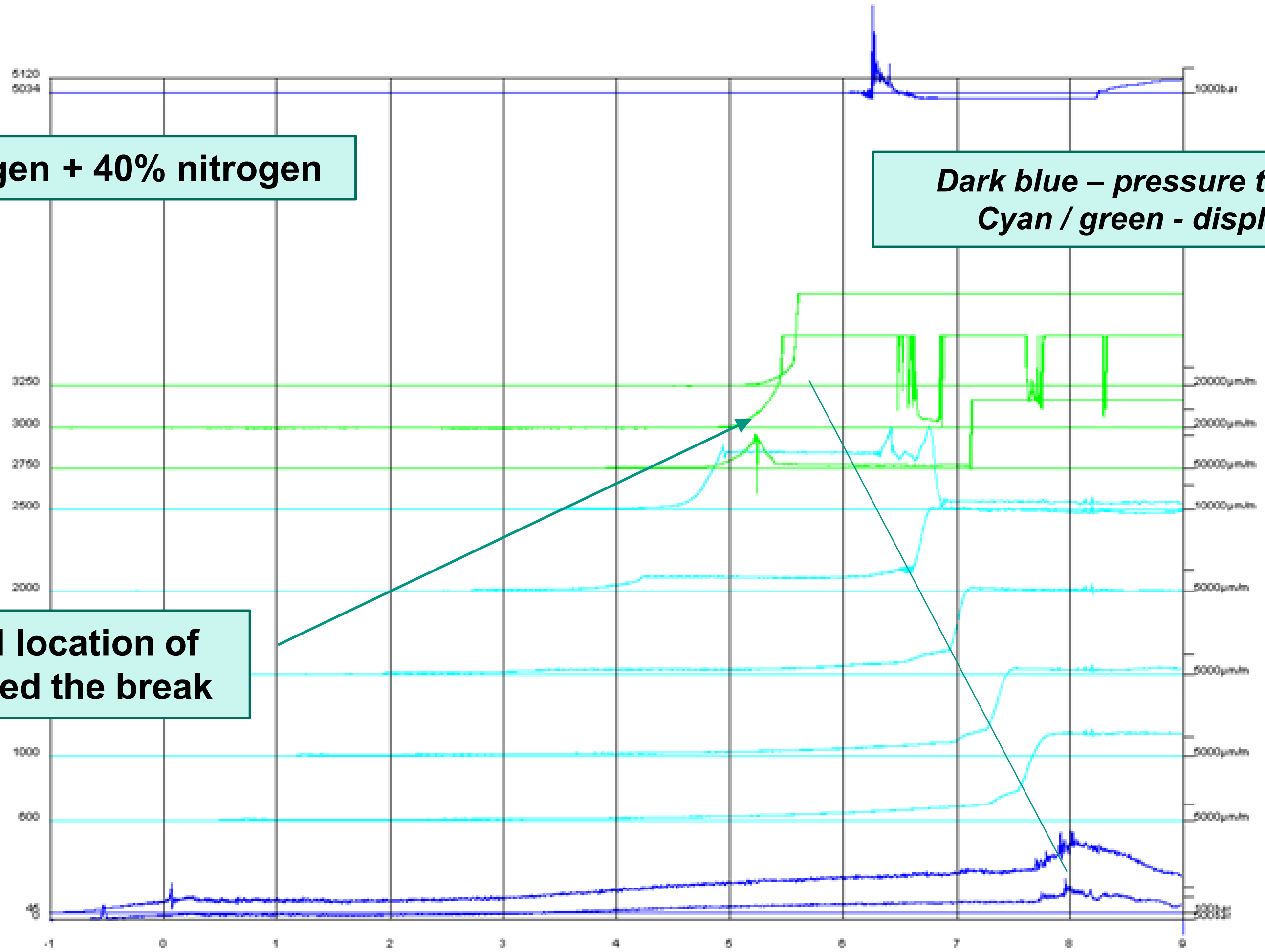
Excessive deformation



Comparison of the residual strain in simulation vs experimental data

Transducer records in test V60E2

Experimental X-t diagram combined DMS & pressure transducers

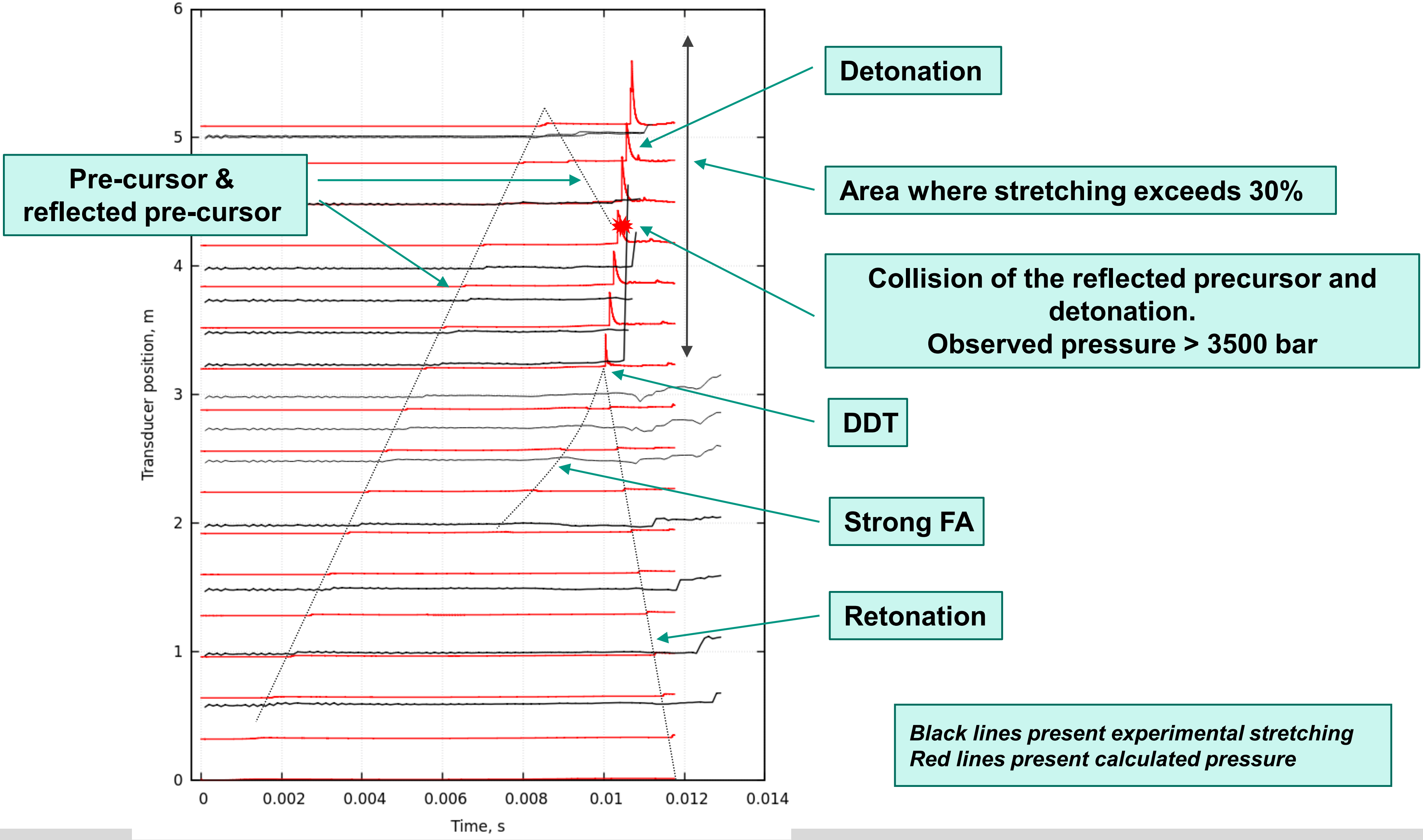


60% oxyhydrogen + 40% nitrogen

Dark blue – pressure transducers
Cyan / green - displacement

Approximated location of the event caused the break

Simulated dynamics for test V60E2



Pre-cursor & reflected pre-cursor

Detonation

Area where stretching exceeds 30%

**Collision of the reflected precursor and detonation.
Observed pressure > 3500 bar**

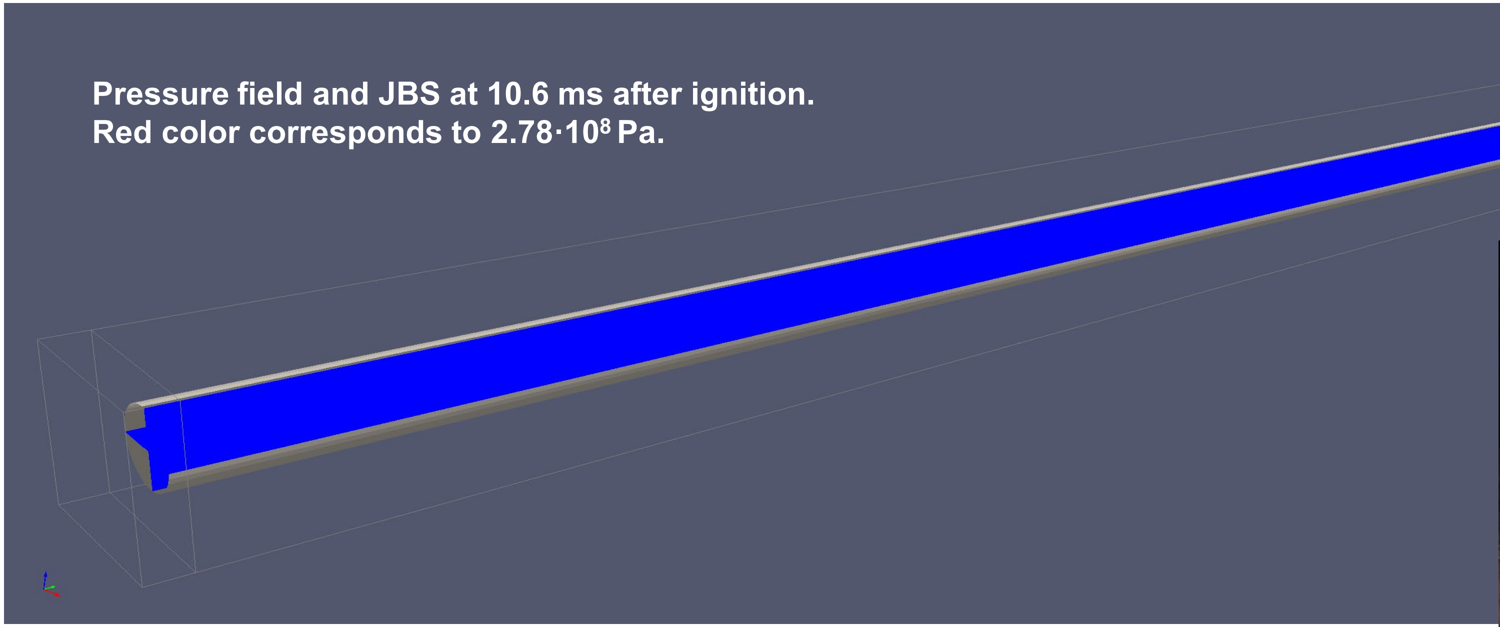
DDT

Strong FA

Retonation

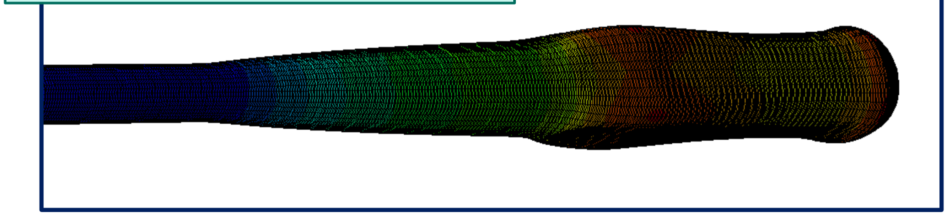
Black lines present experimental stretching
Red lines present calculated pressure

Residual deformation



Pressure field and JBS at 10.6 ms after ignition.
Red color corresponds to 2.78·10^8 Pa.

Residual deformation exceeds 40%



Summary

- New model of dynamic tracking of continuous 2D object (surface) moving in space described by 3D mesh was developed, it was successfully implemented and tested on equidistant mesh. Such technique can be used e.g., for tracking of flame front or interface between different phases.
- The new technique was used for description of exact 3D shape of boundaries moving during process. The model allows realize a real-time data exchange with finite-element code ABAQUS - © Dassault Systèmes to perform coupled gas-dynamic and material stress analysis.
- Using the new model, three simulations based on the experimental data were carried out with the obtained numerical results demonstrating 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.