FSI with Detailed Chemistry and their Applications in LS-DYNA® CESE Compressible Solver

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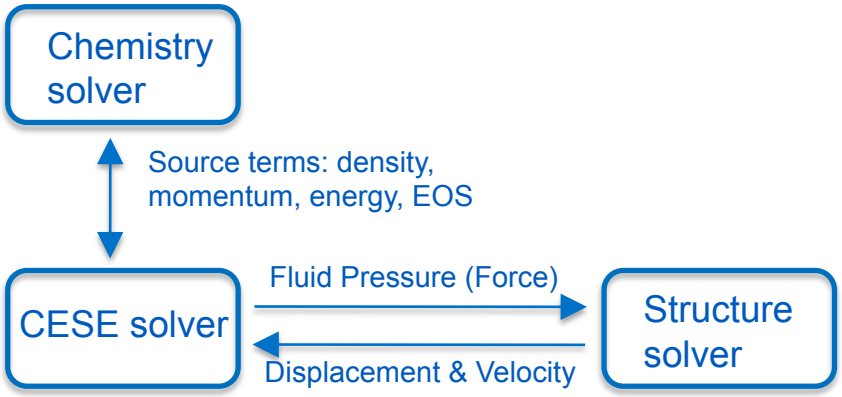
Current Capabilities

- **CESE FSI:**
  - 2D, 2D axis., and 3D Euler solver : SMP, and MPP
  - 2D, 2D axis., and 3D N-S solver with conjugate heat transfer : SMP, and MPP
  - FSI with cavitation (not validated)
  - Applications: Blast and shock wave interactions, Automotive airbag simulation, and Compressible flows with structure interaction.
- **With Chemistry (50 species):**
  - 2D, 2D axis., and 3D Euler Solver : SMP and MPP.
  - Not completed, but partially working at 2D, and 3D N-S Solver with conjugate heat transfer: SMP and MPP.
  - Applications : Offshore plant application (Blast relief wall), Nuclear containment explosion and structure deformation, Inflator + airbag modeling via. CESE FSI solver, Gases explosions interacting with structures.

CESE IBM FSI Solver Coupling

❑ Solver couplings:

In CESE IBM FSI solver, the fluid equations are solved using the CESE method and the solid structural equations are solved by the LS-DYNA® FEM program, while for the elements near the fluid-structure interface it is treated with the direct forcing immersed boundary method, plus the ghost fluid method. The fluid solver gets the displacements and velocity of the interfaces from the structural solver and feeds back the fluid pressures to the structural solver as external boundary conditions. The chemistry solver communicates with CESE solver by exchanging all source terms in conservation equations.

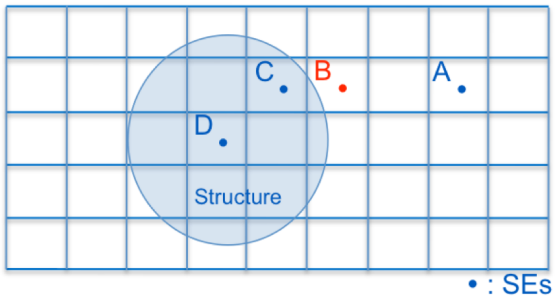


Coupling diagram

CESE IBM FSI Procedure

❑ Calculation procedures:

1) The meshes should be generated separately for the fluid and the structure.
2) Calculate the shortest distance from the structure boundary to an individual solution element (SE) point. Using the distance, the SE points can be separated as the inner fluid one (A), nearby fluid point (B), ghost fluid point (C), or potential fluid point (D).
3) Solve the solid structural equations using the LS-DYNA® FEM solver.
4) Get the updated fluid-structure interface location and interface velocity from the structural solver.
5) Update the shortest distances (only for the near interface SE points) to get a new inner fluid point, nearby fluid point, ghost fluid point classification.
6) Solve the inner fluid points using the CESE scheme.
7) Solve the nearby fluid points using direct-forcing IBM.
8) Apply the ghost fluid method to the ghost points for the next time step.
9) Feedback the fluid pressure to the structural solver.
10) Go back to step 2 until the termination time is reached.



CESE FSI Setup

- Keyword file

❑ Solver selection:

*CESE_CONTROL_SOLVER

$ icese	iflow	igeom	iframe	imixd	idc	isNaN
200	1	3	0	0	0.0	1

- EQ. 0 : fixed Eulerian
- EQ.100 : moving mesh FSI
- EQ.200 : immersed boundary FSI

❑ Time step selection:

*CESE_CONTROL_TIMESTEP

$ iddt	cfl	dtinit
1	0.5	1.0E-8

❑ CESE control parameter selection:

*CESE_CONTROL_LIMITER

$ idlmt	afla	beta	epsr
0	2.0	0.5	0.25

α ↑ : more dissipasive

β ↓ : more smooth

ε ↑ : more stable, but less accuracy

*** alfa : the weighting parameter, beta: $0.0 \le \beta \le 1$, and epsr: the relaxation parameter.

Chemistry Setup

- Keyword file

*CHEMISTRY_MODEL

$ model_id	jacsel	errlim
10	1	0.0

methane20.inp

therm.dat

thran.dat

(N-S solver: μ(k), κ(k), and D(k))

```
!Reduced methane mechanism
!19+1 species and 52 reactions
!
ELEMENTS
O  H  C  N
END
!
SPECIES
CH4     H2      H       O       O2      OH      H2O     HO2
H2O2    CH3     CO      CO2     CHO     CH2O    CH3O    C2H3
C2H4    C2H5    C2H6    N2
END
!
REACTIONS     CAL/MOLE
H+O2<=>O+OH                   1.590E+17    -.927   16872.17
!
!Third body reaction
H+OH+M<=>H2O+M                8.400E+21   -2.000        .00
H2/ 1.90/ O2/ 2.60/ H2O/9.50/ CO/2.60/ CO2/2.60/ N2/ 2.60/
!
!Pressure dependent reaction
CH4(+M)<=>CH3+H(+M)           7.050E+16   -0.558  104891.64
     LOW  /  1.190E+35   -4.911   106959.57/
     TROE/   .555   405.62  4580.87 /
    .
    .
    .
END
```

First 7 set : low term.(200~1000)

Second 7 set : high termp. (100-6000)

$C_p(k)$, H(k), and S(k) are calculated

$$\frac{C_{pk}}{R} = a_{1k} + a_{2k}T_k + a_{3k}T_k^2 + a_{4k}T_k^3 + a_{5k}T_k^4$$

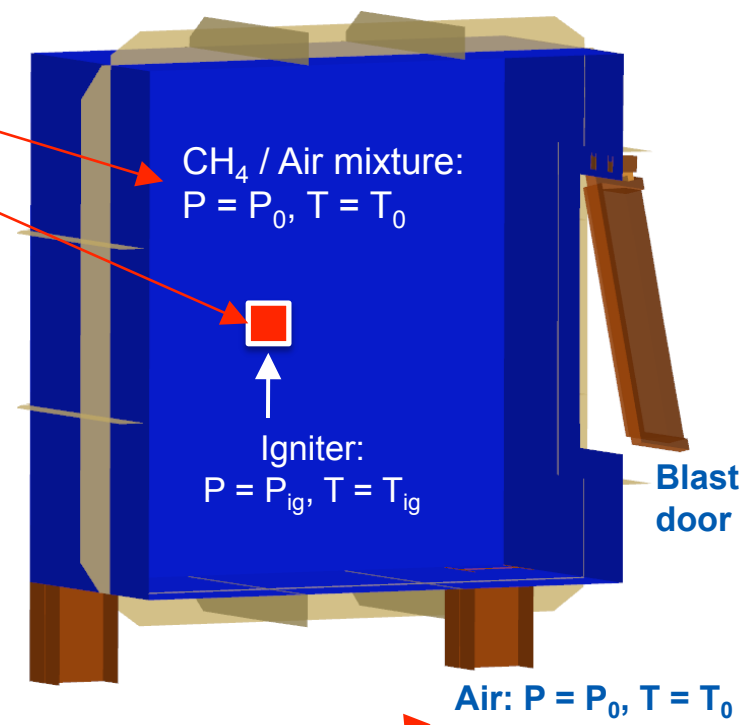
$$H_{pk} = \int_0^{T_k} C_{pk}\,dT + H_k(0)$$

```
THERMO ALL
   200.000  1000.000  6000.000
CH4     RRHO       g 8/99C  1.H  4.   0.   0.G   200.000  6000.000 1000.        1
 1.91178600E+00 9.60267960E-03-3.38387841E-06 5.38797240E-10-3.19306807E-14    2
-1.00992136E+04 8.48241861E+00 5.14825732E+00-1.37002410E-02 4.93749414E-05    3
-4.91952339E-08 1.70097299E-11-1.02453222E+04-4.63322726E+00-8.97226656E+03    4
```

Chemistry Setup

- Keyword file

```
*CHEMISTRY_COMPOSITION
$ comp_id   model_id
       12         10
$ mole_no   species
      1.0       CH4
     8.86        O2
     33.3        N2
*CESE_INITIAL_CHEMISTRY_SET
$    sol_id   comp_id
        5        12
$ initial_conditions
  …
*CHEMISTRY_COMPOSITION
$ comp_id   model_id
       11         10
$ mole_no   species
      1.0        O2
     3.76        N2
*CESE_INITIAL_CHEMISTRY
$    sol_id   comp_id
        5        11
$ initial_conditions
  …
```



Chemistry Setup

- Keyword file

```
*CHEMISTRY_CONTROL_FULL
$     sol_id        errlim
          5           0.0
$
*CESE_CHEMISTRY_D3PLOT
$  model_id
           10
          CH4
           H2
           CO
          CO2
          H2O
$ the followings are not used
*CESE_PART
$       pid         mid      eosid
          7           7          5
*CESE_EOS_IDEAL_GAS
$    eosid          cv         cp
          7           7          5
*CESE_MAT_001
$      mid          c1         c2        pr
          7   1.458E-6       10.4      0.72
```

- *CHEMISTRY_CONTROL_0D
- *CHEMISTRY_CONTROL_1D
- *CHEMISTRY_CONTROL_INFLATOR
- *CHEMISTRY_CONTROL_TBX
- *CHEMISTRY_CONTROL_ZND

Output for the species mass fractions

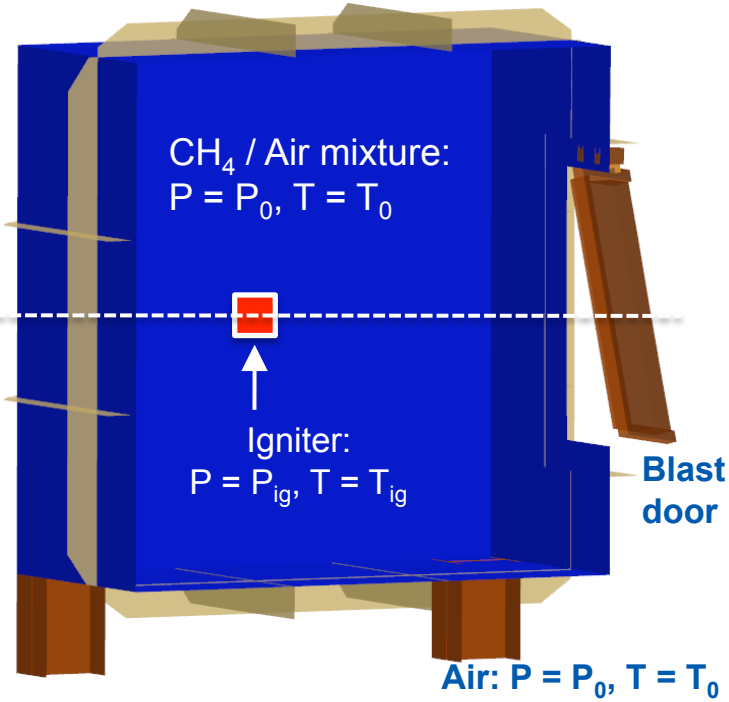
There will be some warning or error message without these parts – we will fix it later on.

Blast Wall Explosion

- **Blast Relief Wall:** *The purpose of the blast relief wall is to vent the combustion gases and pressure resulting from a deflagration an enclosure in offshore plants, so to minimize the human injuries, structural, and mechanical damages.*

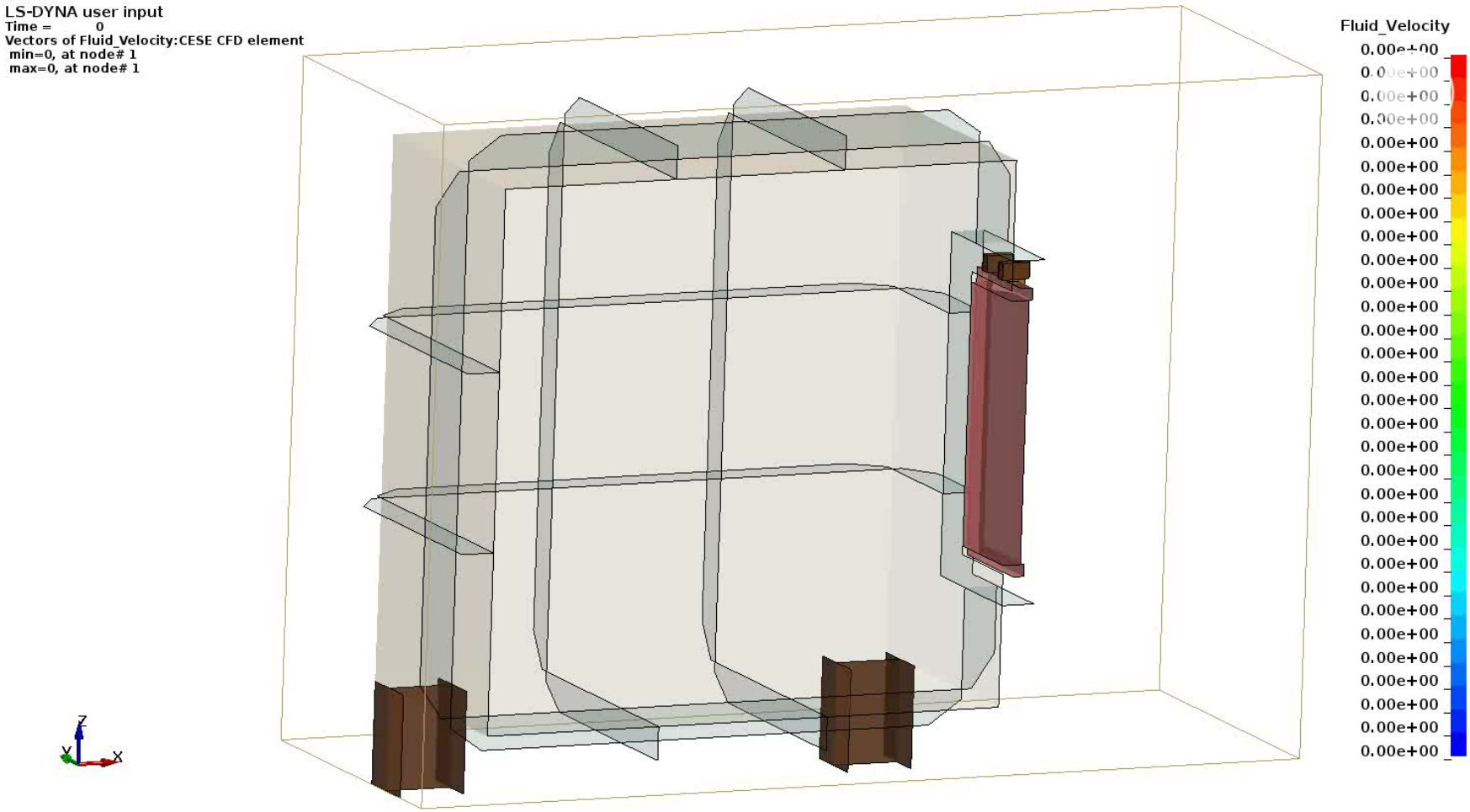
- Mixture : methane(CH4) 10%, and air 90 %.
- The area of the relief wall is 0.399 m^2 with SUS 316 and a cube volume is 4 m^3.
- An electric igniter of 100 J is set at a third of the centerline.
- 20 species, and 52 reaction systems including pressure dependent reactions are employed.
- After 40 ms, the wall opening angle was 12.8° (Exp. : 13°, error ≈ 1.5%)

a) Experimental Model



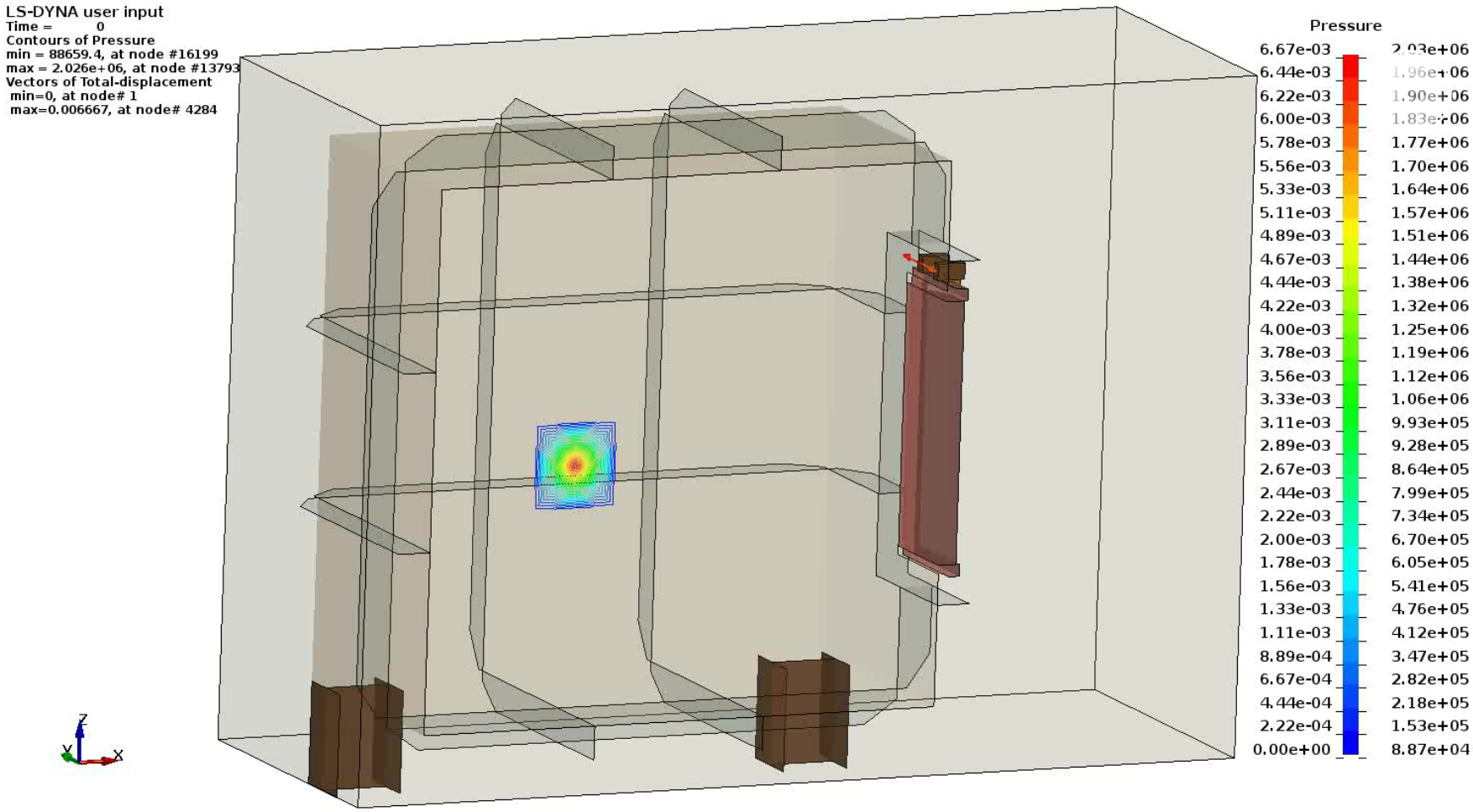
b) Computational Model

Animation : Velocity



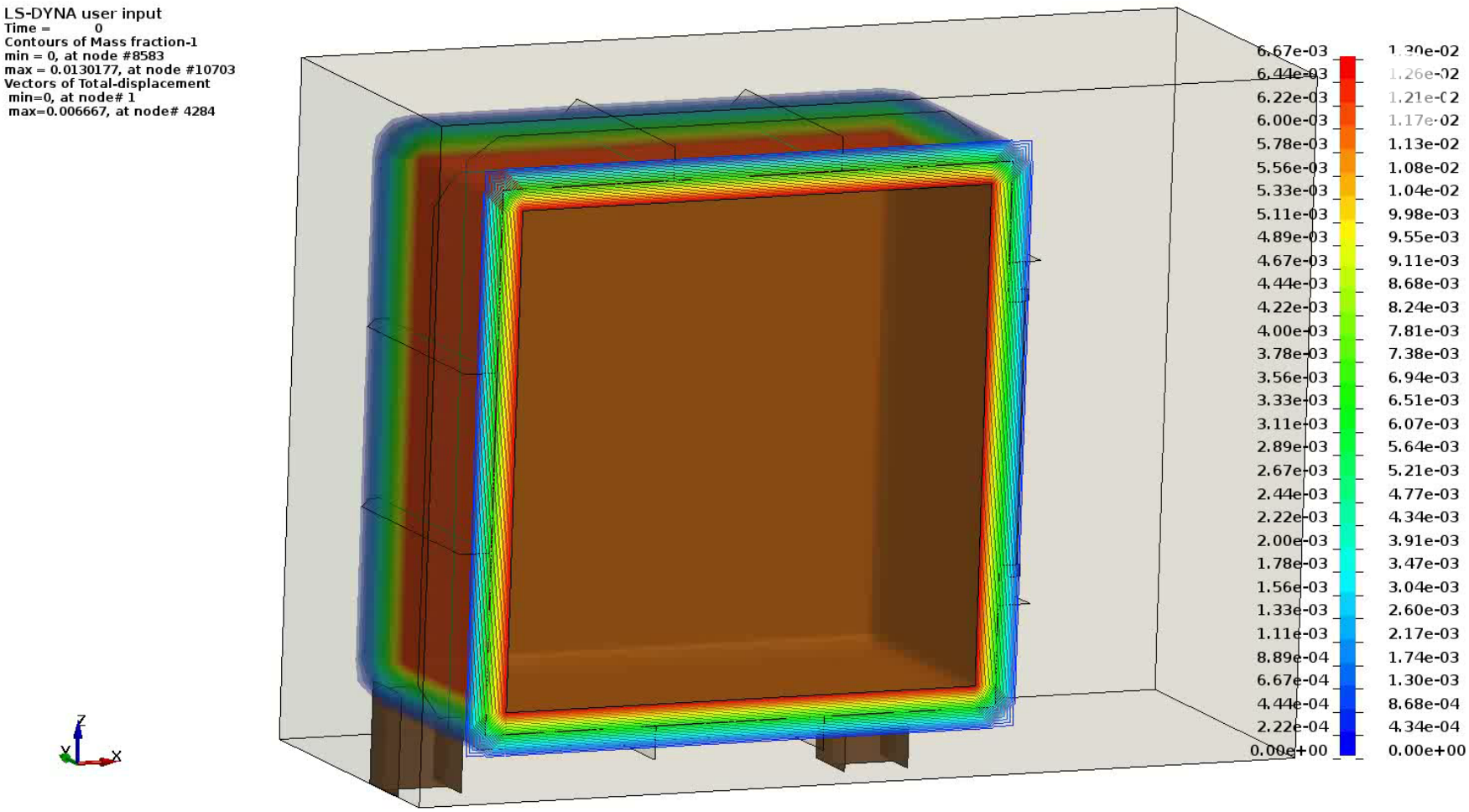
Velocity vectors

Animation : Pressure



Pressure contours

Animation : CH4 Mass Fractions



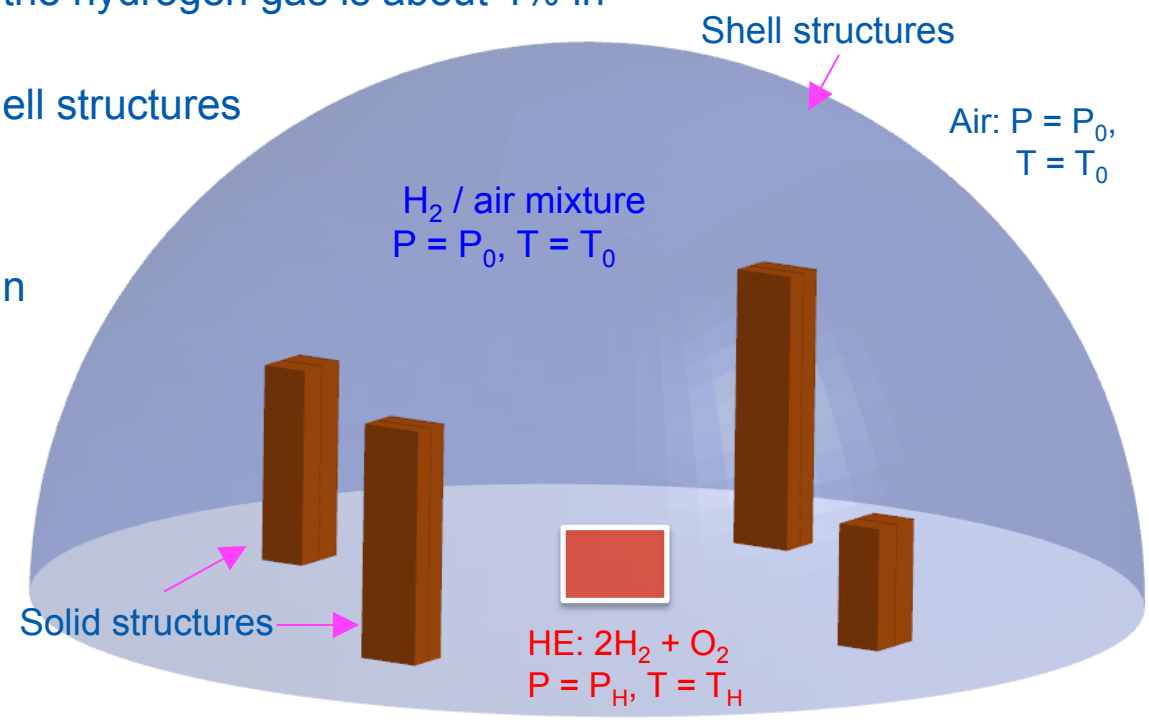
Mass fractions

Shell and Structure Fracture by Gas Explosion

❑ Hemispherical Containment Model

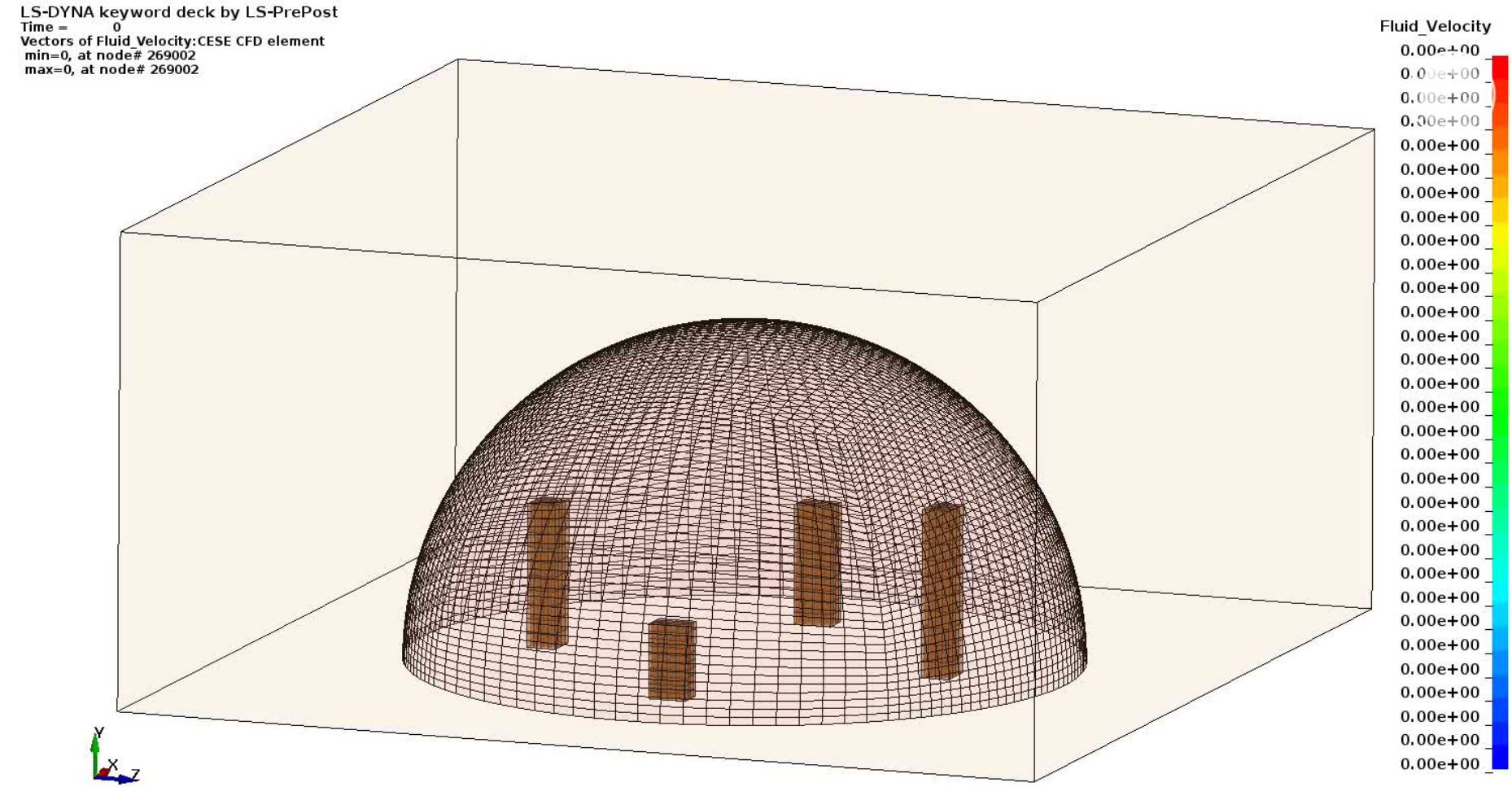
- Hydrogen explosion may happen due to the failure of the cooling system in the nuclear facilities.

  for example: $Zr + 2H_2O \longrightarrow ZrO_2 + 2H2$
- The lower flammable limit of the hydrogen gas is about 4% in terms of the volume fraction.
- The model consists of the shell structures on the dome surface and solid structures inside.
- High explosives are located in the center position with 30 MPa and 300 K.
- The damages will propagate into the internal structures and outside walls.



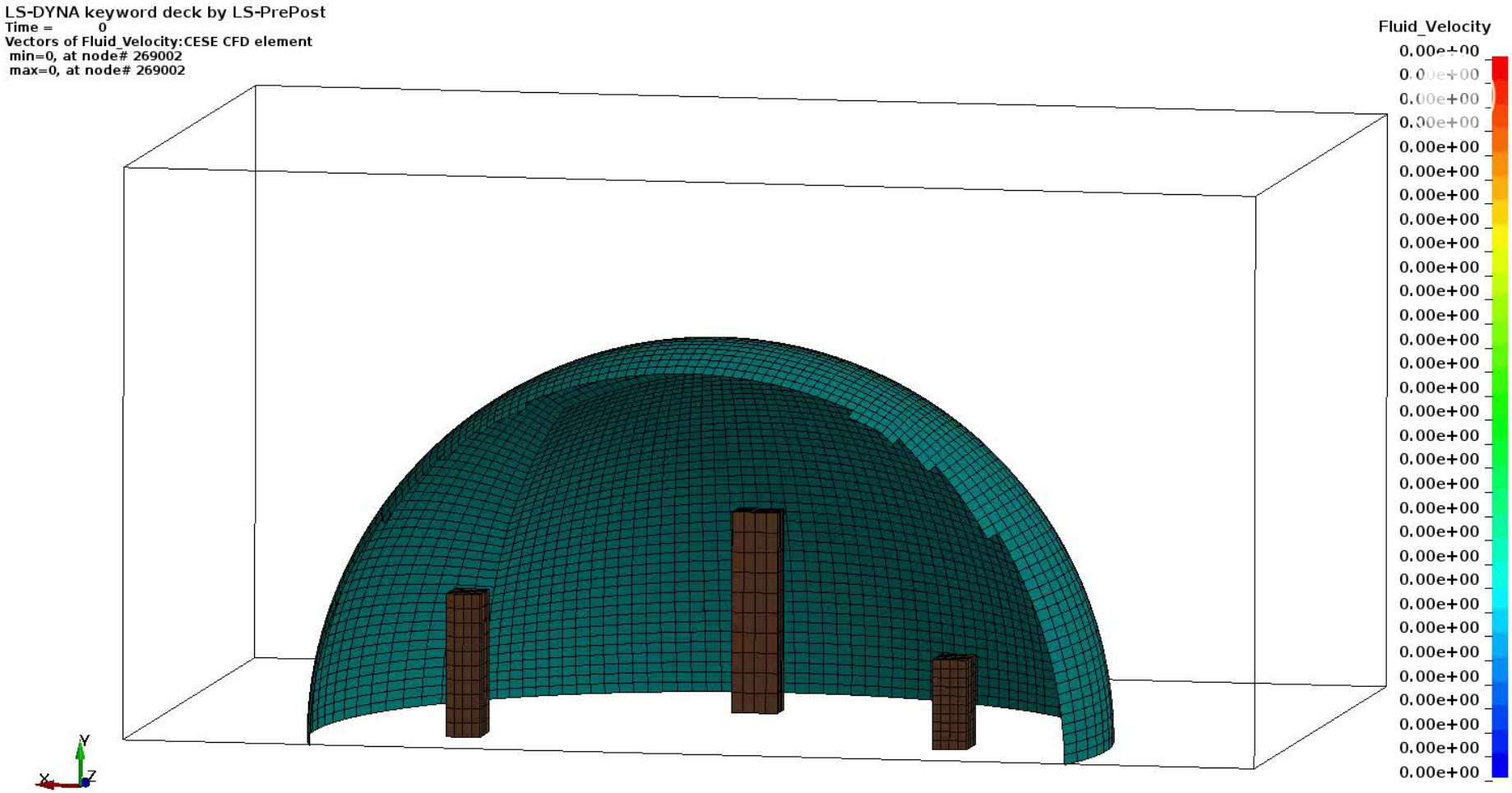
Computational Model

Animation : Velocity



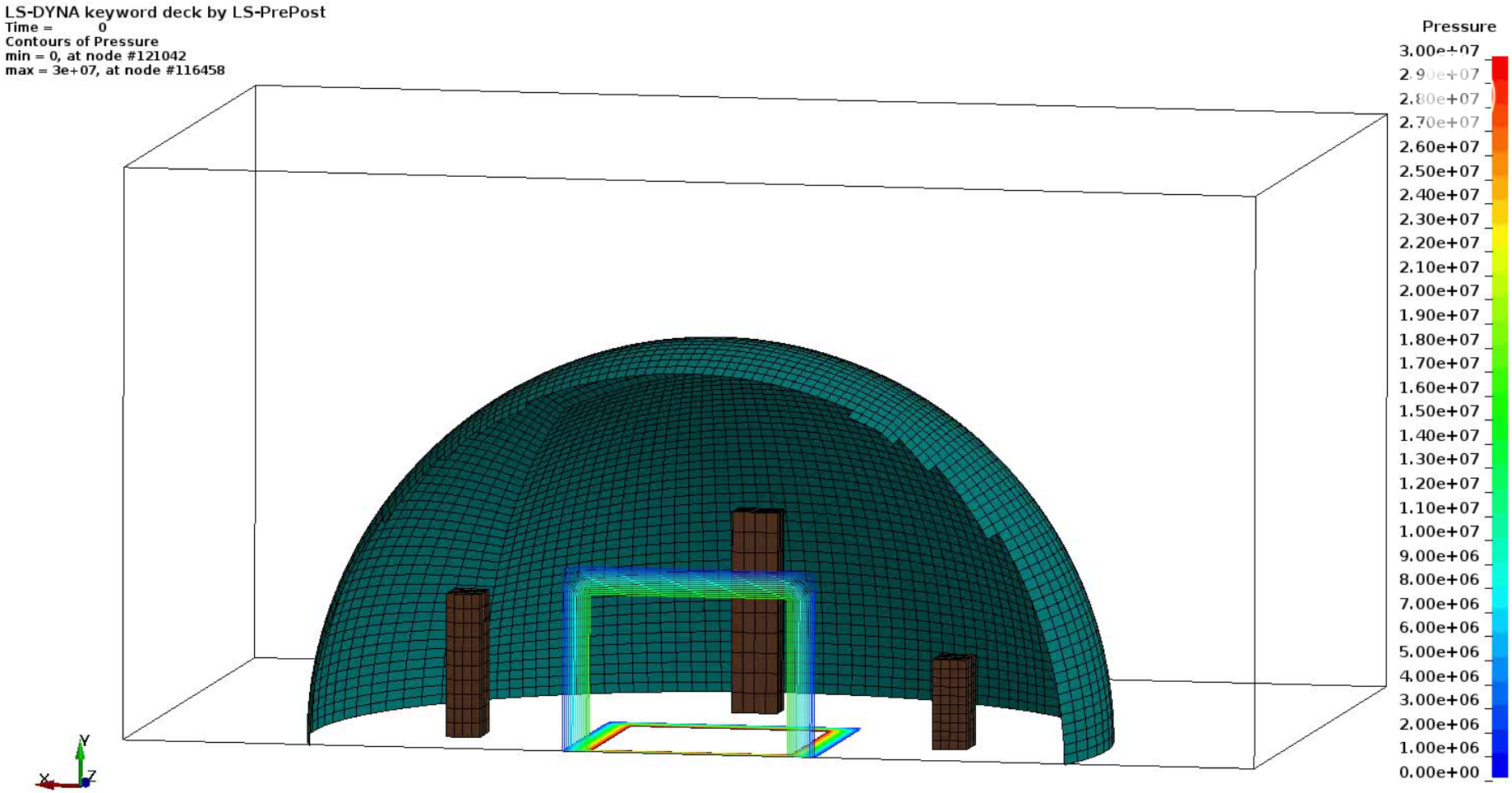
Velocity vectors

Animation : Velocity (half section)



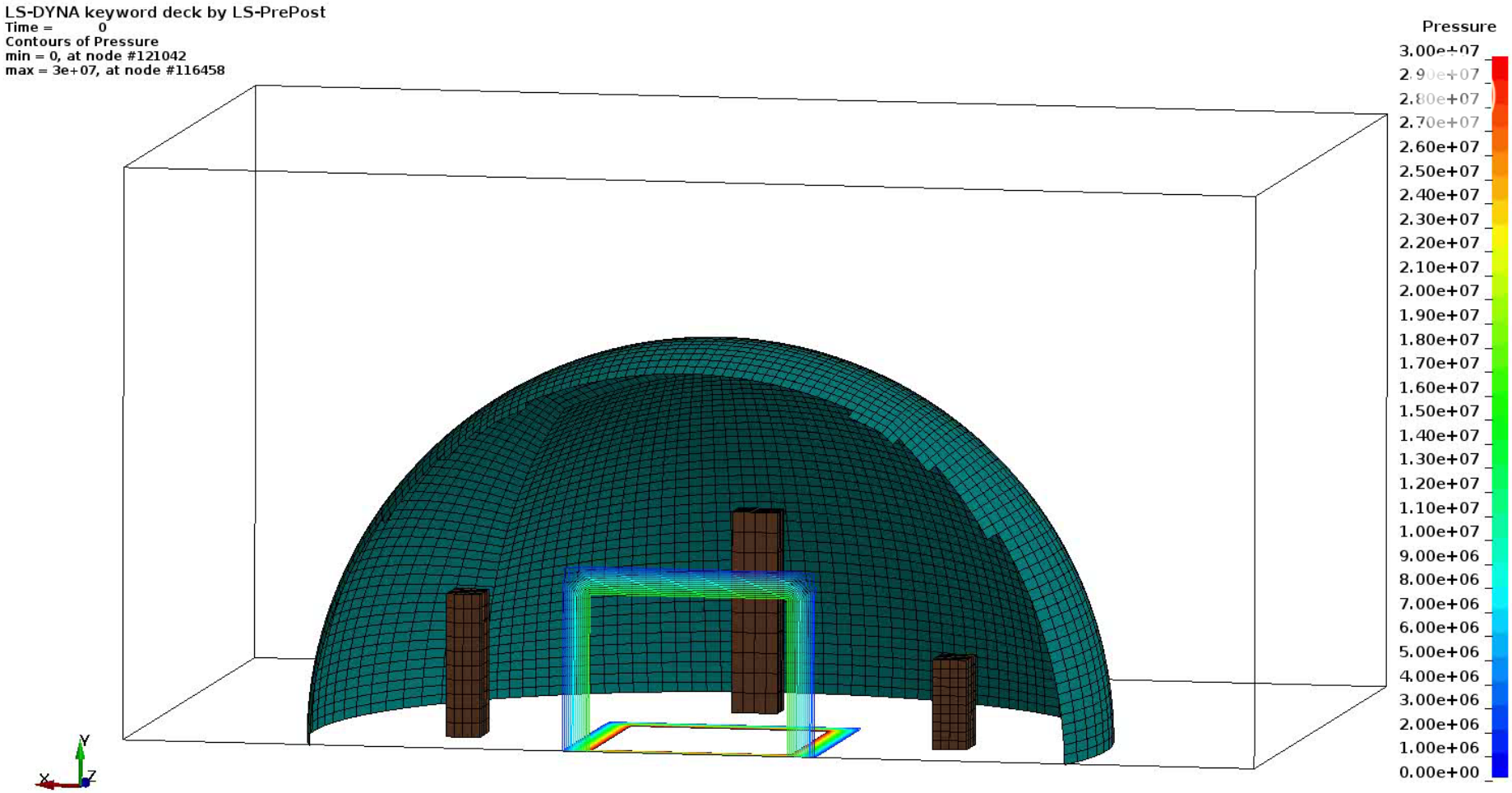
Velocity vectors

Animation : Pressure (half section)



Pressure contours

Animation : Temperature (half section)

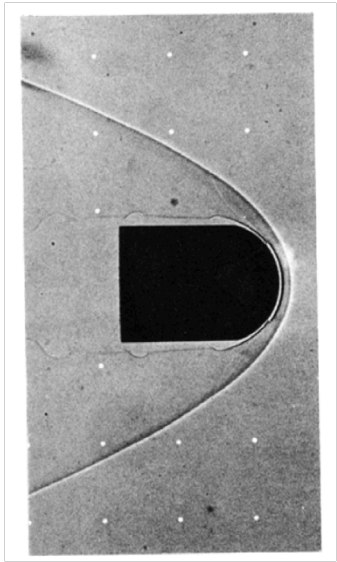


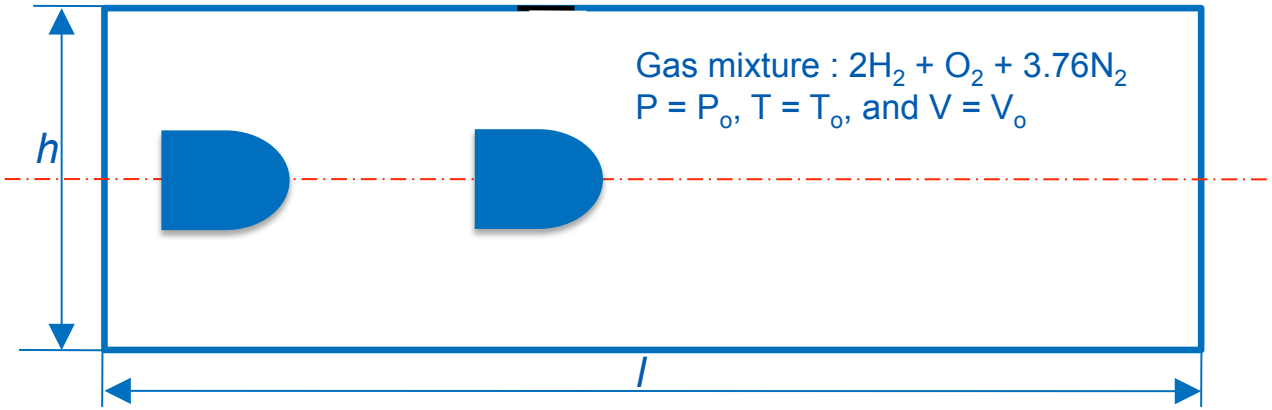
Temperature contours

Shock Induced Combustion by Bullet Acceleration

❑ Shock-Induced Combustion:

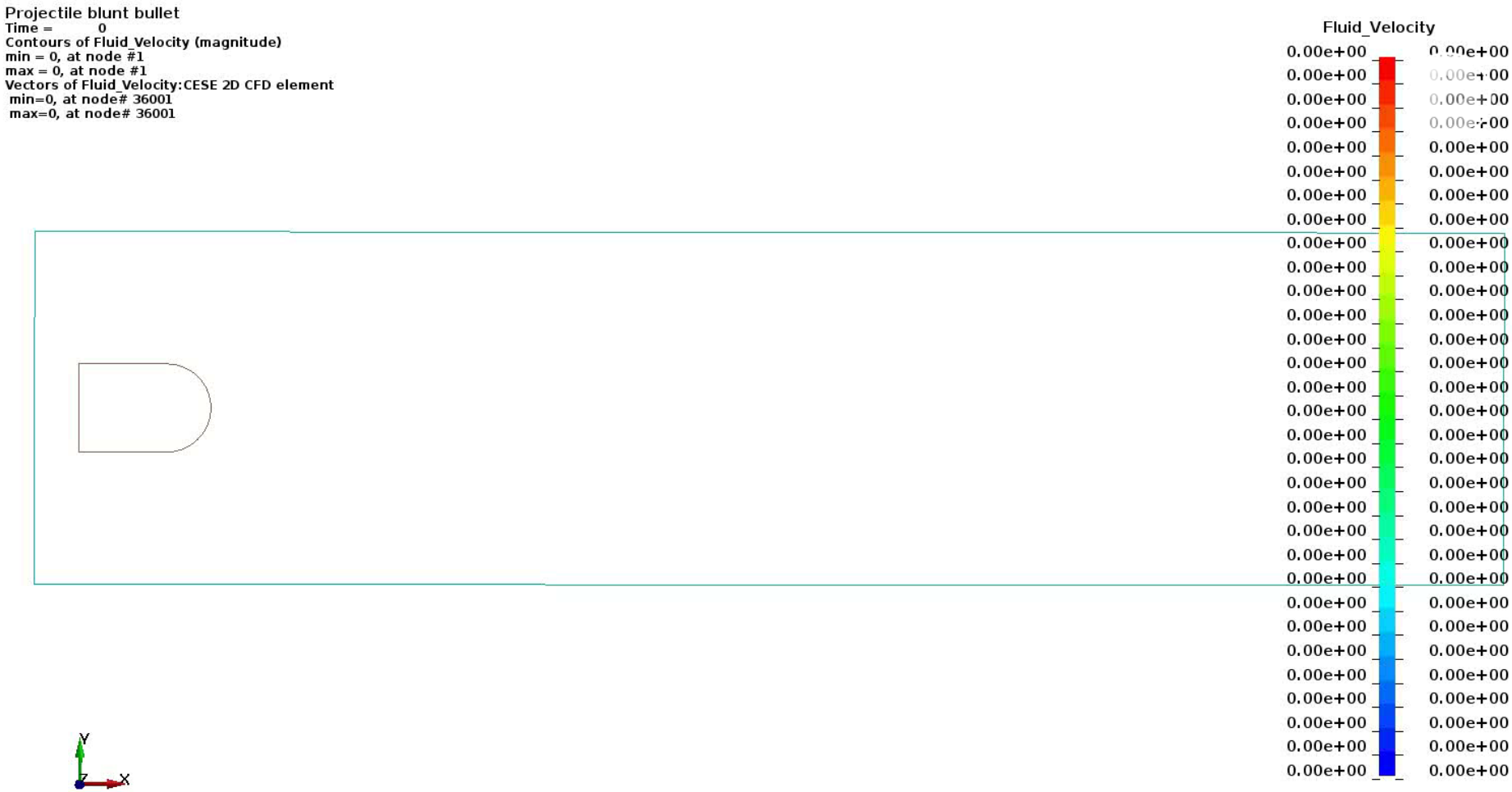
- Hartmuth F. Lehr, Astronautica Acta Vol. 17, pp. 589-597, 1972.
- The bullet is flying with velocities above the detonation velocity of the gas mixture.
- A stoichiometric hydrogen/air mixture with initial conditions.
- The reaction starts near the centerline showing a shock-deflagration system.
- Very difficult FSI problem with chemistry





Computational Model

Animation : Velocity



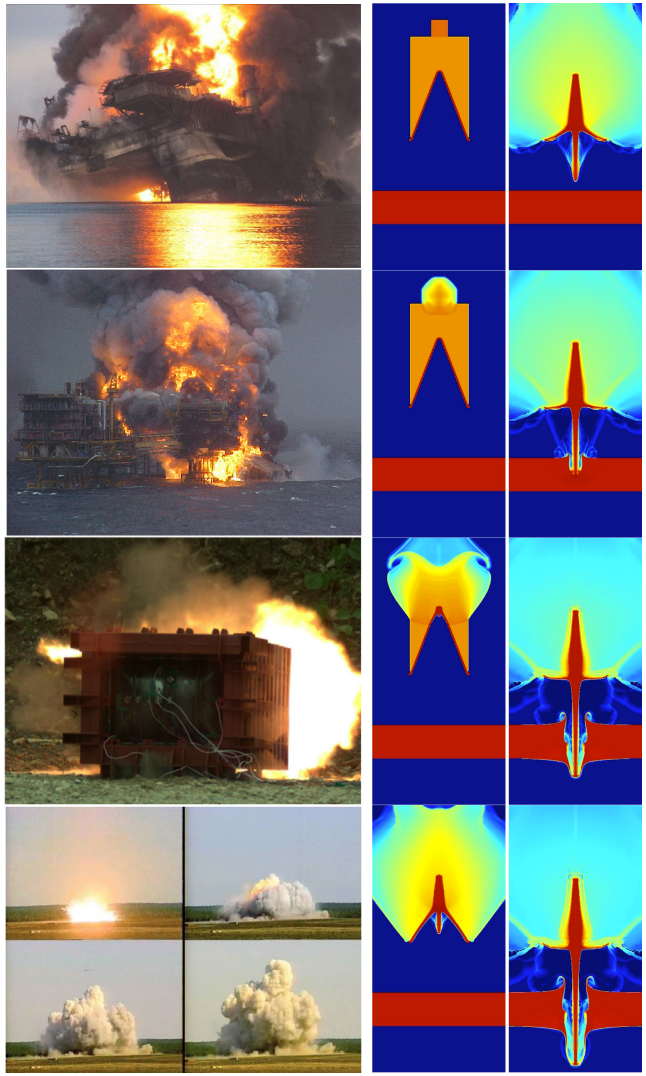
Animation : Pressure

Future Developments

- **FSI with chemistry:**
  - High energy explosions
  - Heterogeneous combustion with structure.
  - Seat belt pretensioners (?)
  - Electrochemistry (battery or bio-sensor)

- **FSI with cavitation:**
  - Cavitating flow with erosion.

- **Load Balance with particle and spray flows:**
  - MPP version of the particle and spray flows
  - FSI with stochastic particle and liquid spray



Thank You !

http://ftp.lstc.com/anonymous/outgoing/ksim/examples/FSI_ibm/LSTC_2017_05_European