Calculation of Blast Loading on a Containment due to an Internal Air-Hydrogen Detonation

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Summary
Hydrogen can be released in the reactor containment after a loss of coolant accident and the probability of the occurrence of a detonation is not negligible.

The paper describes a method of calculation of detonation waves in confined spaces and in particular the overpressures at the the walls.

As a first step one dimensional calculations are presented and compared to analytical results.

Next two dimensional calculations in a containment geometry, starting at two different initiation points, are compared to literature results.

1. Physical Problem and Hydrogen Formation

   During a nuclear accident, large amounts of hydrogen can be released in the containment.
   A detonation of hydrogen may cause a severe damage to the containment and internal structures. By now, there is no evidence that such a detonation cannot occur.

   As a matter of fact, in the case of French containments, if the released hydrogen is perfectly mixed with the ambient air and steam, the resulting concentration is too low to initiate a detonation. Therefore, detonation can occur only if local accumulation of hydrogen is possible.

   Accumulation depends on the thermal hydraulic conditions prevailing during and after the LOCA (thermal stratification), and on the mass flow rate of hydrogen released. By now, there is no proof that accumulation is impossible.

   A similar conclusion can be drawn concerning the deflagration-detonation transition. Recent tests have shown that small obstacles can turn an initial deflagration into a detonation.

   The topic of the paper is the calculation of a blast loading in a confined volume. The code used PLEXUS is briefly described in part 2.

   Validation tests are given in part 3 and a two dimensional calculation in a containment geometry is given in part 4 and compared to existing results /4/.

2. Numerical Model

   We present briefly the computer program PLEXUS for fast dynamic analysis.

   Paper "PLEXUS: A general computer program for the fast dynamic analysis" /3/ gives more details on the code and presents the various possibilities of structures and fluid mechanics calculations.
It is a general program using the finite element method with an explicit time scheme (implicit schemes can also be used but for our detonation problem, it is more convenient to use an explicit scheme).

In the Lagrangian formulation, an automatic remeshing is available.

Any constitutive law can be used, i.e.: perfect gas, mixture of perfect gases, two phase flows.

For boundary conditions, a special treatment is employed: we can write our condition as

\[ C_u = d \]

where \( C \) is a matrix coefficient,

\( u \) a displacement,

and \( d \) the right hand side member.

They are treated by an implicit algorithm via Lagrange multipliers.

In our formulation, the detonation can be considered as a shock front associated to a chemical reaction. Let us consider the mixture composed of perfect gases for which the reaction is:

\[
2 \text{H}_2 + (\text{H}_2 \text{O})_{\text{steam}} + 3/2 \text{N}_2 \rightarrow 3(\text{H}_2 \text{O})_{\text{steam}} + 4\text{N}_2 + Q
\]

The reaction is supposed to be adiabatic and exothermic (37 kcal released for one mole of created water) and also that the thermodynamic parameters are independent of the temperature.

The reaction is initiated at a threshold temperature \( T_L \).

The initial temperature is 327.6°K and it is necessary to give a relation between propagation velocity \( v \) and the difference \( \Delta T \) between the initial temperature and the threshold, i.e. for \( v = 1,980 \) m/s, we obtain \( \Delta T = 15°K \) therefore the threshold temperature is 342.6°K.

The calculations have been performed with Lagrangian formulation.

3. One Dimensional Calculations - Validations

Two one dimensional detonation calculations have been performed in plane and axisymmetric geometry. The results of the plane case are compared to the Chapmann-Jouguet theory. The axisymmetrical case put in evidence the focusing effects of the shock waves.

a) Definition of the test calculation:

We used a stoichiometric mixture. The concentration of components is:

hydrogen: 28%  
oxide: 9.4%  
nitrogen: 13.1%  

The initial pressure is 1.63 bar and the tube is 1 m long.

One hundred mesh points have been used with initiation in the second mesh point.

The walls are supposed to be rigid (at \( x = 0 \) and \( x = 1 \) for the plane case, at \( r = 1 \) for the axisymmetrical case).

b) Results of test case A:

We can see in figures 1, 2 and 3 the propagation of the wave as a function of space at three different times. On figure 4, the pressure is given as a function of time for five space locations: \( x = 0 \), \( x = 0.01 \) m, \( 0.5 \) m, \( 0.8 \) m and \( 1 \) m.

Figure 4 shows the two sweeps way and back of the shock wave, the overpressure at the first reflexion and the residual pressure.
These results can be compared to the theoretical prediction. 

According to the Chapmann-Jouguet theory, we have in an infinite medium where

\[ \frac{P_2}{P_1} = 2 \frac{\gamma_2 - 1}{\gamma_2 - 1} \frac{Q}{C_v T_1} \quad \text{and} \quad \frac{P_3}{P_1} = 4 \frac{\gamma_2 - 1}{\gamma_2 - 2} \frac{Q}{C_v T_1} \]

\( P_1 \) is the pressure of the unburnt gases
\( P_2 \) the overpressure (C-J point)
\( P_3 \) is the pressure of the burnt gases.
\( \gamma_1 \) and \( \gamma_2 \) are the adiabatic expression constants of the burnt and unburnt gases and \( Q \) the heat of the reaction.

Thus \( \frac{P_2}{P_3} = 2 \frac{\gamma_2 + 1}{\gamma_2 - 1} = 2 \) if \( \gamma_2 = \gamma_1 \)

The agreements with the results of figures 1, 2, 3 is good.

If we suppose that the initial pressure \( P_1 \) is negligible compared to \( P_2 \) and \( P_3 \), the overpressure at the wall is given by:

\[ \frac{P_3}{P_2} = \frac{5\gamma_2 + 1 + \sqrt{17\gamma_2^2 + 3\gamma_2 + 1}}{4\gamma_2} \]

where subscripts 1, 2 and 3 are defined in the figure above.

For \( \gamma_2 = 1.4 \), we obtain \( \frac{P_3}{P_2} = 2.54 \). If \( P_2 \) is equal to 20 bars, then \( P_3 = 50.7 \) bars. The agreement with the results of figure 4 is reasonably good.

c) Results of test case B:

In figures 5, 6 and 7, we can see the propagation of the shock wave at the same times as for figures 1, 2 and 3.

Figure 8 is the equivalent of figure 4 for the axisymmetric case.

It can be noticed that the overpressure at the wall at the first impact of the shock wave is similar to that obtained in case A, while the overpressure is considerable at \( r = 0 \) when the shock wave returns to the center. The focusing effect can be encountered in reactor containments.

4. Two-dimensional Calculation in a Containment

It has been showed /4/ that focusing effects and multiple reflections can lead to important overpressures in a containment.

Moreover, the containment load is very sensitive to the location of the initiation point (cf /4/). We wanted to check these conclusions by running the same calculations as those of reference /4/.

The definition of the test case appears in figure 9 with the mesh used.

The results are shown in figures 10 and 11 for an initiation at mid height (35 m above...
the ground) and in figures 12 and 13 at the bottom.

The pressure histories at selected points on the wall (see figure 9) are shown in figure 14 for the first case and in figure 15 for the second one.

We can see that for a source located at 35 m, the effects are similar at all the points. But if we put a source in the bottom, the pressure histories are similar except at the apex of the dome where the overpressure is 1.5 time the value obtained for the previous case.

Another feature can be pointed out: the first peak is not less important than the following ones. The secondary reflexions are as much damageable at the first time in spite of the fact that they occur without chemical reaction in a completely burnt atmosphere.

5. Conclusion

The PLEXUS code seems to be well suited to the calculation of shock waves in confined volumes.

The one dimensional calculations are in good agreement with the theory. Qualitative agreement has been found with existing calculations in a two dimensional containment geometry. Nevertheless, the problem of the possibility of occurrence of a detonation remains opened.

Bibliography

/1/ LANDAU & LIPSCITZ, Mécanique des Fluides, Ed. MIR.