Numerical Simulation on DDT in Real and Large Scale Combustion Chamber Using a Combustion Velocity Model and Ignition Model with a Detailed Chemical Reaction System

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1 Introduction

It is a current situation that a few real and large scale numerical analysis and experiment of deflagration-to-detonation transition (DDT) has been found out. Such large scale calculation is necessary to the field of aerospace, space science, nuclear power system, weather, and so on., but since it costs a lot, the problem is that the high quality calculation is not much. The present study will be conducted numerically on a large scale DDT using the recent new computational techniques. Especially, a numerical analysis is performed using hydrogen/air mixtures to validate a large scale DDT experiment. The correspondent experiments were conducted at the Kurchatov Institute, Russia in 1998-2001[1-3]. The data obtained at Kurchatov Institute are compared with the present numerical simulation.

The DDT data obtained in the RUT facility have been compared with the study performed by Breitung et al.[4] and then, Vollmer et al.[5] in 2012 and Hasselberger[6] in 2015. Their numerical results have clear difference with the RUT experiments. Especially, their numerical DDT distances are close to the

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experimental ones, but their DDT time have some shorter times than the RUT data. These differences are caused probably by their unknowing the detailed RUT facility's size and configuration. The present work will make a clear reason why such difference occurs between the numerical results and the RUT experimental ones.

2 RUT experimental system configuration and its main results

The experimental facilities of Kurchatov Institute are shown in Figs. 1-a and b.

Fig.1-a RUTfacility

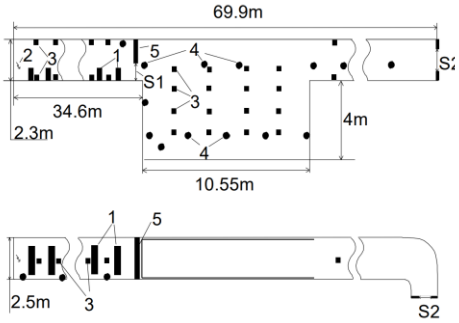

Fig.1-b : Experimental configuration. Total volume is 480 m3. 1 - obstacles; 2 - ignition position; 3 - pairs of light flow transducers; 4 - pressure transducers; 5 - steel plate.

2.1 Experimental conditions

In Fig.1-b, the ignition plug location is at the left end wall 40 cm from the floor and 12.5 cm from the left wall: six obstacles before the ditch are situated 10 cm from the floor: and these obstacles with their blockage ratio (BR) of 60 % are set at 50 cm from the left wall and 0 cm from the right wall toward to the downstream. Firstly, the numerical calculation starts with the ignition plug which sticks together at the left wall and secondly, it starts with the ignition plug which is set at 12.5 cm from the left wall. The results of those numerical simulations will be described later.

The numerical result of induction time to detonation in the case at the initial conditions of the left wall-sticked plug show some different from that of the experimental result (which will be explained later). Then the location of ignition plug is set at the second case, which is closer to the experimental condition and described above in Fig.1-b. The experimental result is shown in Fig.2 as follows:

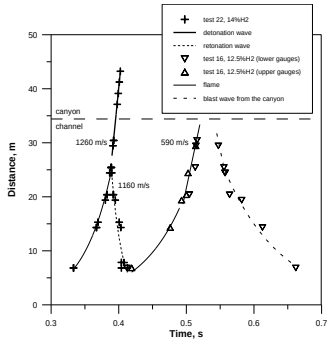

Fig.2 Propagation of the flame and pressure waves for DDT in the channel (14% H2) (and DDT in the canyon (12.5% H2)).

3 Numerical method and results

3.1 Numerical method

The present numerical calculation is performed using FOCUS-i which is developed by AdvanceSoft company and its details are described in Table 1.

Table 1 Detailed numerical methods

Item	Contents
Scheme for advection term	**3rd-order MUSCL TVD + AUSM-DV**
Evaluation for first-derivative	**Gauss's theorem**
Time integration	**Runge-Kutta formulas**
Turbulence model	**k-ω SST[7]**
Laminar flame velocity	**Cantera[8]**
Turbulent flame velocity	**Dinkelacker's wrinkling model[9]**
DDT	**Ettner's model[10]**
Ignition delay time	**Cantera with UT-JAXA[11]**
Chemical species ratio of burnt gas	**NASA-CEA[12]**

3.2 Some of numerical model and chemical reaction mechanism

Some of key models in the present FOCUS-i code are :

(i) Laminar flame velocity: this is calculated using Cantera code.
(ii) Turbulent model: $k-\omega SST$
(iii) Dinkelacker's wrinkling flame velocity model

3.2.1 Dinkelacker's Wrinkling flame velocity model[9]

This model is developed by Dinkelacker and is a function of Lewis number (Le) which originally varies as follows:

$$\Xi = 1 + \frac{0.46}{Le} Re_t^{0.25} \left(\frac{u'}{S_{L_0}}\right)^{0.3} \left(\frac{p}{p_0}\right)^{0.2}$$

where $Le = \frac{Sc}{Pr} \approx 1.0 \sim 1.38$. Later, variable Le number is applied.

3.2.2 Initial flame and boundary condition

The initial flame of 1 m radius is set at the center between the ceiling and floor of the tube (Fig.3-a), but the DDT time is shorter than 320 msec than the experimental one. Hence, as described earlier, the initial flame position is moved to the location which is more similar to the experimental one (Fig.3-b). The results for those conditions are discussed at the next chapter 4.

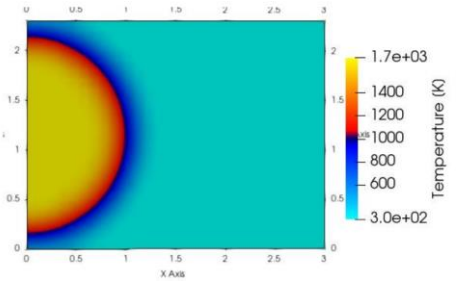

Fig.3-a Ignition location A of the first try

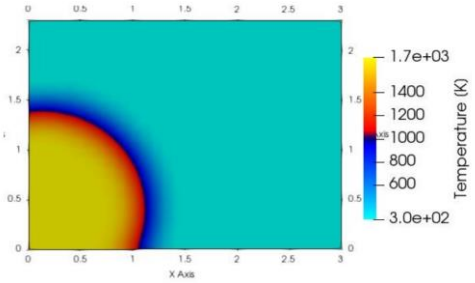

Fig.3-b Ignition location B of the second try

3.2.3 Calculation of chemical reaction

The detailed chemical reactions of hydrogen/air consist of nine species and 10 to 25 elementary reactions, but, in the case of large numerical system by such as direct numerical simulation, it is very costly and needs a long time calculation. Then the numerical method recently used is applied in the present simulation, which is that the species fraction, reaction progress, and other thermodynamic data for temperatures and pressures are calculated in advance and are stored as a big data. Whenever we need such data, we can get them by giving temperature and pressure. In this way, we can save the calculation time and cost pretty much. The chemical reaction model we used is UT-JAXA reaction mechanism[11] which is not only good for high temperature, but also good for high pressure, like detonation atmosphere.

4 Results and discussion

In order to perform a numerical calculation of H_2/air DDT with obstacles in a large and real size combustion chamber such as RUT facility, a validation study is performed for a large scale numerical analysis.

4.1 Comparison between RUT22 experimental results[1-3] and numerical calculation ones

Many numerical calculations conducted up to now have, more or less, not solved the initial and boundary condition problem. In other words, many studies took the simple models for those conditions such as a simple chemical reaction mechanism, simpler ignition location and ignition energy, simpler boundary condition for obstacles. Hence, their numerical results do not match with the experimental data. The present study will show such difference and will get the better results comparing with the experimental one of RUT22.

4.1.1 Numerical results of DDT in RUT22 for two different initial and boundary conditions

As describing at 3.2.2 Initial flame and boundary condition, in the first try of calculation, the ignition point locates at the left wall surface and the center between the ceiling and the floor. But the second try of calculation, the location of the ignition point is not attached to the left end wall, but 12.5 cm away from the wall and its height is 40 cm from the floor. Those conditions are similar to that of RUT22 at Kurchatov Institute. The difference of numerical results between two conditions are shown in Figs.3-a and -b, Fig.4, and Fig.5.

As seen from Flame velocity of Fig.4 and x-t diagram of Fig.5, the first ignition location case does not give DDT and the second one gives DDT. From those results, there can be two major problems: one is that why the first case did not get DDT and the second case didit; and why the second case has an early DDT time of 320 msec comparing with the experimental result.

In the first problem of whether DDT occurs or not, DDT looks occurring even the first ignition location. But its DDT distance is much longer and does not appear in Fig.5 because there might be data at such long distance.It is difficult to figure out why the first case needs longer induction length. It seems that the first ignition location has less fluid dynamic effects than the second ignition location.

The second problem of earlier DDT occurring comes from the initial ignition condition. It is not shown in this manuscript, but the dealing of initial flame energy and momentum condition may have such problem. The flame size of 1 m is dealt in the present problem, but as far as energy consumption, energy by velocity must be accounted when the flame becomes 1 m size. However, so far, the energy by velocity does not considered at this moment. When we calculate roughly the energy by velocity, the DDT time becomes about 300 msec longer, then we can see that the DDT time becomes almost similar to the experimental one.

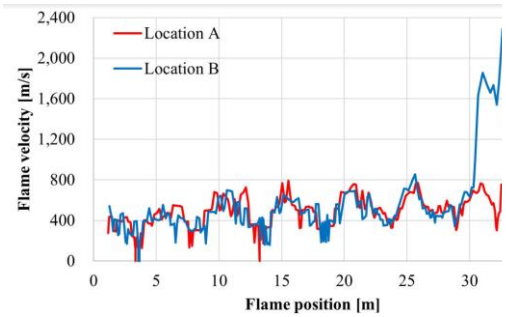

Fig.4 Flame velocity at flame location

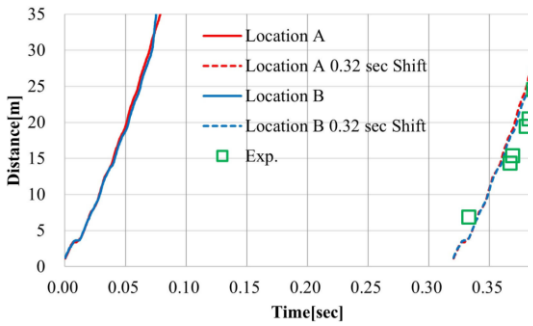

Fig.5 Flame velocity at flame location

5 Conclusion

The numerical analyses of DDT in the large and real size obstacle combustion tube were performed and the results were compared with the ones experimentally obtained at the RUT22 system in the Kurchatov Institute. As a result, the ignited flame becomes detonation and non-detonation depending on the initial condition and the boundary condition.

As for the DDT time, the numerical results has 320 msec shorter than that of experimental ones, but when the initial and boundary conditions are considered more carefully, we recognized that this time difference of 320 msec will disappear.

After a little more study on such treatment of numerical conditions, the developed code will be used for the real cases.

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