Numerical Study on Hydrogen/Air DDT in a Large Scale Channel: physical and chemical models and initial and boundary conditions

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1 Introduction

Large-scale experimental systems have not been performed worldwide because of their size. One of the few such large experiments is the one in Kurchatov Institute, Russia, RUT experiments in 1996-2001[1], and its data are used for the numerical validation of nuclear reactors and others. Large computer systems have been developed recently to deal with such big systems. However, many of those numerical analyses have not obtained good data due to the mis-setting of initial and boundary conditions, as well as physical and chemical models. However, those researchers concluded that their results were positive. For example, some papers [2,3] show that 2D simulation gives a better DDT time than the 3D case. Our original simulation gave results similar to the ones above. Dr. Chaumeix [4] gave us a suggestion to calculate this problem in our private communication, so that we may get the velocity profile between the ignition point and the first obstacle, and then we will get the answer. She said she had a similar experience when she calculated a problem. Some of the researchers, who had a similar problem, slid the numerical results since their flame speed matched the experimental data.

Hence, we decided to simulate a large system of the RUT experiments in more detail. First of all, we like to confirm the developing code in detail, which is a validation by comparing it with experimental data. As many researchers did, we picked up the RUT experimental results to match with them. The following procedure is considered, as shown by Chan and Thibault [5]:

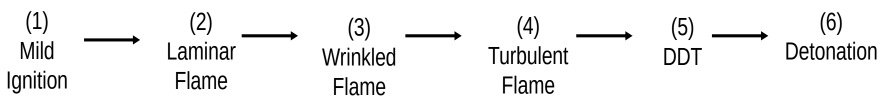

Fig.1 Process of ignition, flame propagation, DDT, to detonation [5]

where Fig. 1 shows six processes from ignition to detonation. To develop the code to explain the physics, each step must be understood well. We must prepare the conception of each step with equations and

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models, which must be integrated, however, we have to check whether those equations and models are appropriate or not. For example, this time, we used Ettner's DDT model (2013) [6], then we checked it carefully. Because of the above discussion, we applied several integration systems. Then we will finally obtain a better and correct result.

2. Numerical method

The governing equations for DDT simulation are three-dimensional compressible Reynolds-averaged Navier-Stokes equations (FOCUS-i program [7]) with 9 species and 21 elementary reactions of the H2-air reaction mechanism. The TVD Runge-Kutta method is used for time integration, and the third-order TVD and AUSNDV schemes are used for the convection terms. The Green-Gauss method is used for viscous terms. The cell-centered Finite-Volume method is used for discretization. The G-equation is used for the combustion model. The κ-ε SST model is applied for the turbulent model. As said before, Ettner's ignition delay time model [6] is used for the detonation transition model. Laminar flame velocity is calculated by the Cantera code [8], and turbulent flame velocity is obtained from Dinkelacker's wrinkling model (2011) [9]. The ignition delay time data table is obtained using the Cantera code and UT-JAXA reaction mechanism [10]. Thermophysical properties of each chemical species are calculated using the NASA polynomial, and species concentration is done by NASA-CEA [11]. MPI is used for parallel computing, and a GUI is applied for data acquisition. The time step is about 1 μs, and the grid sizes using the AMI method are between 2.5cm and 20cm, depending on the combustion condition. The total grid number is about 3.76 million.

Ettner's DDT model (2013) [6] is simply explained here that the model introduces the auto-ignition information to the production term of the flame front model to use the rough grid resolution. By using this way, the number of grids can be kept at about several million, although the large computational field of 35m is applied. The Ettner model is used by several research groups to understand its usefulness, such as Ettner,2013 for DDT in a 5.4 m wind tunnel [6], Ettner, Vollmer, Sattlemayer, 2014 for DDT in about 35m tunnel [12], Wieland et al., 2021 for DDT in 2.9-6.3m wind tunnel [13], Nakamori and Kirihara, 2022 for DDT in a 5.4m wind tunnel [14].

2.1Numerical conditions for a numerical simulation of a large-scale DDT (RUT22)

A RUT experiment at Kurchatov Institute, Moscow, Russia[15] (Fig.2) was performed in 1989. In

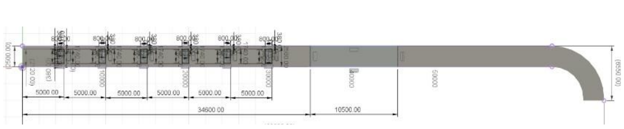

Fig. 2 Experimental configuration of the test RUT22 at Kurchatov Institute,

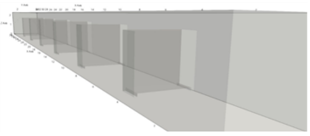

Fig. 3 Three dimensional configuration of the RUT22 experimental facility (Numerical configuration).

this tunnel, six obstacles are lined up for 34.6 m, and the canyon (pool) of 10.5 m, which is not included in the simulation. In the RUT22 experimental facility. DDT can be seen depending on its initial condition.

The horizontal length of the obstacle is 200cm, its width is 80cm, the space between obstacles is 450cm, and the space underneath of obstacle is 10cm. Almost all configurations of the Test facility of Test 22 do not have the spaces underneath and horizontal space to the wall of obstacles, which are 10cm and 50cm, respectively. These spaces are important for the flame propagation dynamics and provide different results for the numerical simulations depending on the situation.

In other words, the flames go through such spaces faster than those in the mainstream. Then DDT occurs differently from the results without the spacing problem in any numerical simulation. Another discrepancy occurs when the correct ignition condition is not set. Many researchers know those problems, but because of the computer performance, capacity together with, and time-consuming problems, most of them might skip solving those problems. We did not use a big supercomputer to solve such large-scale numerical simulations, but used a typical-sized computer that medium-class companies can afford.

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(1) The position of the ignition is set on the left wall of the tube at the lower half of its height. This flame configuration is obtained from a 3D H_2/air spherical flame calculation, together with its 2D cross-section fitted with the wall.

(2) The hydrodynamic instability of a flame proposed by L. D. Landau and E. M. Lifshitz (Fluid Mechanics, 2nd Edition, 2013) [17] may provide a better effect on flame dynamics in the present problem. This hydrodynamic instability has recently been modified as "a Fractal model", but the authors dare to use the idea of hydrodynamic instability of a flame by Landau and Lifshitz.

Other numerical conditions for the RUT22 simulation are:

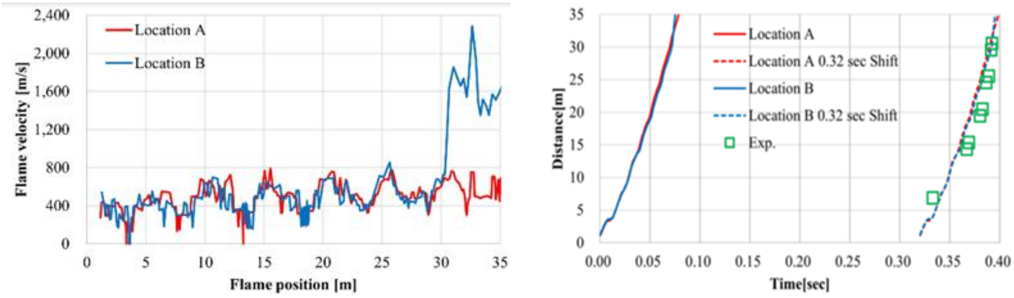
(a)H_2 concentration condition: 14% H_2 with air; (b) Flame size and configuration; First a spherical flame was calculated numerically; (c)Initial temperature and pressure: 298 K and 0.1Mpa; (d)Initial spherical radius: 100 cm; (e)Initial ignition position: x=12.5cm, y=125cm, z=40cm; (f)Number of obstacles: 6; (g)BR(blockage ratio): 0.6; (h)Total number of grids: 375, 793; (i)Boundary conditions for walls: non-slip and iso-thermal.

3. Numerical results

Numerical simulations are performed for the detonation case of the RUT22 experiment. The numerical results are discussed based on the sequential developments for better correction, which are (1) the location of the ignition point and (2) the consideration of self-similar of turbulent combustion.

3-1 The location and configuration of the ignition point

There are many reasons that the results of numerical simulation cannot agree with the experimental ones, which come not only from the numerical problem but also from the inaccurate expression of experimental devices. In the present study, we decided to solve such a problem first to express the correct experimental devices. This is because we found that many researchers simplified the complicated experimental devices. Sometimes such simplification becomes fatal or not too fatal unexpectedly. The present case study may be the latter case. The experiments RUT22 at the Kruchatov Institute show that the ignition position did not attach to the wall and stayed at the middle height closer to the floor, which was placed on the rectangle box. Hence, we decided to set the ignition position at a place similar to the experiment. As a result, DDT occurs when the ignition position is near the bottom floor, but does not occur when its position is at the center of height from bottom and top. As far as DDT is concerned, the case that the ignition position is closer to the experimental one provides a closer result than that it is not. It is also seen in Fig.4 that the flame velocity (Fig. 5-(a), the inclination of x-t diagram) does agree with the experimental one too. However, the position of DDT in Fig. 6-(b) stands up 32 msec earlier than the

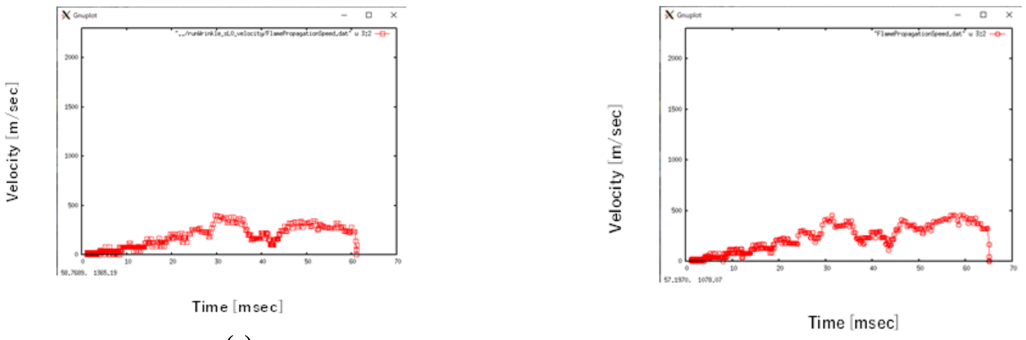


(a) (b)

Fig. 4 Flame velocity and x-t diagram of the flame propagation: Location A is the middle height of the experimental tunnel and Location B is near the bottom floor.

3-2 The importance of the wrinkling model

The wrinkling factor by Dinkelacker [9] is confirmed not to work for this problem itself from Fig. 7, which means the flame does not transfer to detonation, even though the thermodynamics effect of Metghalchi and Keck [18] is considered.



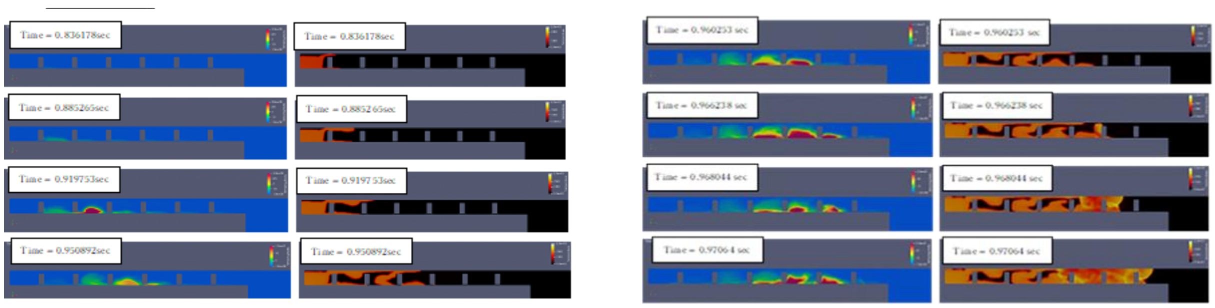
(a) (b)

Fig. 5 Combustion velocity calculated the present problem for the cases of (a) Combustion velocity using only with the Dinkelacker's wrinkling factor and (b) Combustion velocity using with the wrinkling factor and thermos-dynamics effect of Metghalechi and Keck[18].

From the results of Fig. 5, not only the wrinkling factor but also the wrinkling factor together with the thermodynamics effect is considered, DDT did not happen, probably because when turbulence becomes strong, there is a condition of flame velocity increases.

3-3 The consideration of the self-similar law of turbulent flame

For the time being, the ignition problem is solved, but the DDT time distance problem of 32 msec is not solved yet. To this end, since the wrinkle flame model does not trigger much DDT, we investigated



(a) Wrinkling factor (b) Temperature (a) Wrinkling factor (b) Temperature

Fig.6 Time-dependent (a) wrinkling factor profiles vs. (b) Temperature profiles during DDT.

some other phenomenon that works in highly turbulent conditions. Then we paid attention to the idea of Landau and Lifshitz [17]. They talked about the self-similar law of turbulent combustion (SSLTC) (related to hydrodynamic instability in flame) in their book. We thought such turbulent effects were also important for this type of problem. We added the SSLTC model together with the wrinkle flame model. It is known that the SSLTC model provides a better contribution to the turbulent flame.

When flame propagates in the non-obstacle channel, κ and u', produced by RANS, are almost zero. It means that before the flame comes to an obstacle, the wrinkling model almost does not contribute to the flame. However, the SSLTC model also does not contribute momentum and energy to the flame because the flame characteristic length is still small compared to the separation vortex size; the SSLTC model does not change the whole stream.

Hence, when the turbulent strength is small, the SSLTC model affects the flow much, but does the turbulent flow. This is one of the reasons that we decided to throw the SSLTC in the flows. The following is how much the SSLTC model affects the flow.

$$SS\ Factor = S_{L0} C_g \left(\frac{\rho_u}{\rho_b}\right) \sqrt{\frac{t+t^*}{\kappa}} \qquad (1) \qquad \text{where } t^* = \frac{\kappa}{\left[S_{L0} C_g \left(\frac{\rho_u}{\rho_b}\right)\right]^2} \quad \text{and } C_g = 0.002 \quad (2)$$

The wrinkling factor increases with the turbulent intensity and pressure fluctuation. This is because the self-similar law of turbulent combustion (SSLTC) affects the flame. However, the effect of the SSLTC is not much by itself (about 10-20 %). Hence, the combination of the SSLTC with the wrinkling is important.

Figure 7 (SSLTC model only) and Figure 8 (SSLTC model and wrinkling model) show the importance of a combination of the SSLTC model and the wrinkling model. When we compare Fig. 10 and Fig. 11 with the experimental results (the experimental results are found in Fig. 6-(b)), the use of both models provides a closer the experimental results.

Fig. 11 DDT using SSLTC model and wrinkling model

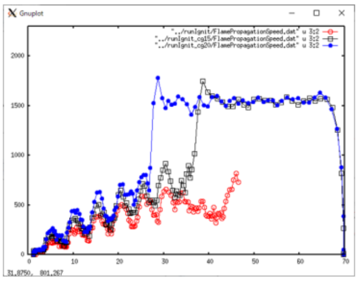


Fig. 7 DDT using SSLTC

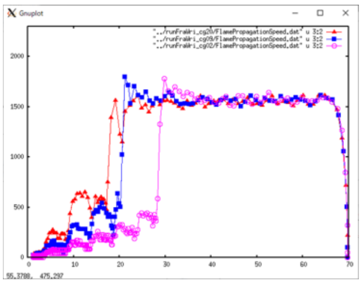


Fig. 8 DDT using SSLTC model and wrinkling model

4. Conclusion

The numerical simulation was performed to figure out the DDT process in the large real-scale combustion tunnel of 34.6 m length and 3x3 m cross-section of RUT22, the Kurchatov Institute, using several physical models. Two important points were made clear: the first is that researchers must set a correct configuration of the ignition system, and the second is that they must use not simple, but appropriate physical models based on the DDT physics. Then, the large-scale system calculation requires more detailed initial and boundary conditions: for example, the gap between the obstacle and the wall must be considered for detonation and DDT problems.

The interesting findings are that the small-scale chamber calculation may not show the difference between the experimental result and the numerical one, but the large-scale chamber calculation may show a large difference between the experimental and numerical results. Hence, a more detailed configuration of initial and boundary conditions must be considered. This difference is related to the detonation cell size, which does not change with the chamber size.

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