NUMERICAL STUDY OF THE DETONATION BENCHMARK USING GASFLOW-MPI

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ABSTRACT

Hydrogen has been widely used as an energy carrier in recent years. It should a better understand of the potential hydrogen risk under the unintended release of hydrogen scenario, since the hydrogen could be ignited in a wide range of hydrogen concentrations in the air and generate a fast flame speed. During the accidental situation, the hydrogen-air detonation may happen in the large-scale space which is viewed as the worst case state of affairs. GASFLOW-MPI is a powerful CFD-based numerical tool to predict the complicated hydrogen turbulent transport and combustion dynamics behaviors in the three-dimensional large-scale industrial facility. There is a serious of well-developed physical models in GASFLOW-MPI to simulate a wide spectrum of combustion behaviors, ranging from slow flames to deflagration-to-detonation transition and even to detonation. The hydrogen–air detonation experiment which was carried out at the RUT tunnel facility is a well-known benchmark to validate the combustion model. In this work, a numerical study of the detonation benchmark at RUT tunnel facility is performed using the CFD code GASFLOW-MPI. The complex shock wave structures in the detonation are captured accurately. The experimental pressure records and the simulated pressure dynamics are compared and discussed.

1. INTRODUCTION

The use of hydrogen as an energy carrier has been increased exponentially in recent years. Due to the high reactivity of hydrogen, it could be ignited in a wide range of volume concentrations in the air and generate a fast flame speed, threating the surrounding humans and industrial facilities. Therefore, it should a better understand of the potential hydrogen risk under the unintended release of hydrogen scenario. Significant progress of hydrogen safety issue has been made with support from international and national organizations, such as the HySafe network (www.hysafe.org) [1-3]. A serious of key phenomena related to hydrogen safety have been identified based on the Phenomena Identification and Ranking Table (PIRT) exercise [1], including the issues of hydrogen transport and distribution, refueling stations and stationary applications, and others. Moreover, the standard benchmarks also have been proposed to validate the physical models in the numerical tools [1]. In the unintended hydrogen release scenario, the hydrogen-air detonation may happen in the large-scale space, which is viewed as the worst case state of affairs. Many efforts have been made to investigate the hydrogen-air detonation behaviour in the large-scale industrial facilities by using the experimental researches and numerical simulations [4-6].

GASFLOW-MPI is a widely-used CFD-based numerical tool to predict the complicated hydrogen turbulent transport and combustion dynamics behaviors in the three-dimensional large-scale industrial facility [7-15]. Its simulation results are well accepted in industrial communities. There are well-developed physical models in GASFLOW-MPI, such as turbulence behavior module, chemical dynamics module and other engineering facility models, to simulate a wide spectrum of turbulent combustion behaviors, ranging from slow flames to deflagration-to-detonation transition and even to detonation [7-9]. The 3-D hydrogen-air detonation of a hemispherical balloon in open atmosphere has been investigated using GASFLOW-MPI. However, the detonation behavior in a confined space has not been performed for the CFD code GASFLOW-MPI. The hydrogen-air detonation experiment based on the RUT tunnel facility within the confined volume is a well-known benchmark to validate the combustion model. In this work, a numerical study of the detonation benchmark at RUT tunnel facility is performed using the CFD code GASFLOW-MPI. The goal is to further evaluate the capability of GASFLOW-MPI in simulating the detonation for hydrogen safety analysis.

This paper is constructed as following: the outline of the RUT facility and the numerical method are introduced in section 2. Section 3 provides and discusses the numerical results by using the CFD code GASFLOW-MPI. The main conclusions are presented in section 4.

2. NUMERICAL SIMULATION OF RUT BENCHMARK

2.1 Outline of RUT Facility

A series of large-scale hydrogen–air detonation experiments were carried out at the RUT tunnel facility at Kurchatov Institute in Russia [4]. The RUT facility is a steel-lined reinforced concrete structure shown in Fig. 1, which was 27.6 m long, 6.3 m deep and 6.55 m wide (maximum dimensions). The volume of the facility was 263 m^3. The HYD05 experiment has been chosen to simulate the hydrogen-air detonation in this paper. It was carried out in homogeneously hydrogen/air mixtures with 20% vol of hydrogen. The initial mixture temperature and pressure were 293 K and 0.1013 MPa, respectively. Mixing was assured by fans as hydrogen concentration and mixture uniformity were checked taking samples from two different points of the experimental volume. The non-uniformity was less than 0.5% vol of hydrogen. The hydrogen-air detonation was initiated at point A in HYD05, as shown in Fig. 1. The detonation was started by direct initiation with a high explosive charge of 200 g weight as the initiator being located at distance 80 cm from the floor and 50 cm from the wall [4].
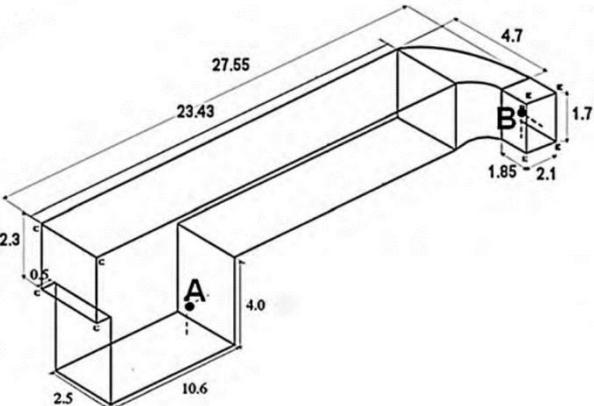

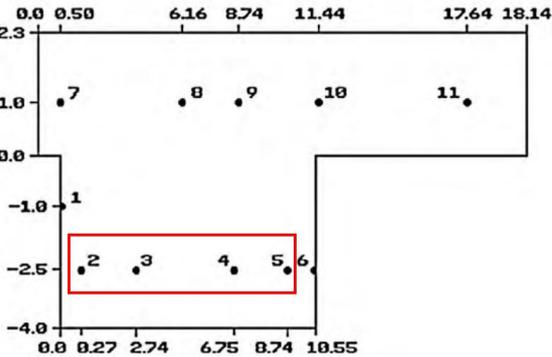Fig. 1. Experimental facility scheme [4]   Fig. 2. Location of the pressure transducers [4]

High-frequency measurement system were used and signal was recorded with a sample rate of 5 μs. Over-all, eleven monitoring points were selected where pressure transducers were used to record pressure-time history, as shown in Fig. 2. The pressure transducers were arranged in two lines inside the experimental volume. The first one was placed in the canyon (lower part of the facility) and
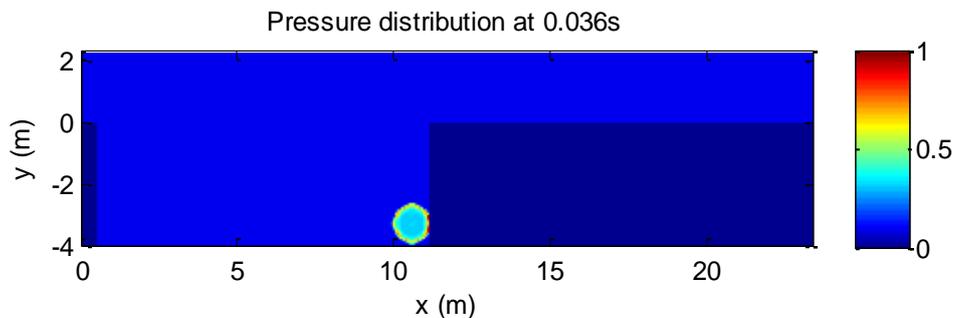
included transducers 1-6 (line 1). The second one was placed in the channel with transducers 7-11 (line 2). The pressure transducer numbers 2-5 were located on the longitudinal wall of the canyon, and the transducers 7-11 on the opposite wall of the channel. Transducers 1, 6, 11 were placed in the middle of the transversal walls. For HYD05 experiment (ignition at point A, close to the sensor 6 in Fig.2), transducers 7-11 are distorted by multiple reflections and are not of interest for the comparison. In this work, the pressure readings from pressure transducers 2-5 are utilized to compare with numerical results.

2.2 Numerical Simulation

In this work, the parallel CFD numerical tool GASFLOW-MPI is employed to simulate this detonation benchmark. The computational domain is 23.45 m × 6.3 m × 2.5 m in x, y and z direction, receptively, with cubic cells at 0.05 m which leads to 2,948,400 Computational Volumes (CVs). The mixture was initially stagnant. Hydrogen and air mass fractions were 0.017 and 0.983, respectively. The initial temperature and pressure condition of mixture were 293 K and 0.1013 MPa. In this simulation, the detonation was initiated by a ignition source with high temperature and high pressure in the region of 0.2 m × 0.2 m × 0.2 m (4 × 4 × 4 CVs). Since an industrial scale facility is simulated, a one-step global chemical kinetics model based on a modified Arrhenius law accounting for local hydrogen and oxygen concentrations is employed to ensure the computational efficiency. The non-slip boundary condition for the momentum equations and adiabatic boundary conditions for the energy equation were imposed at the wall. The second-order Von-Leer numerical scheme is used for the convection terms, which is a kind of TVD schemes to capture the shock wave in the detonation. The second-order central difference scheme is employed for the diffusion terms. The adaptive time step is used whose CFL number is limited to below 0.2. The total computational time is set to 40 ms.

3. RESULTS AND DISCUSSIONS

The simulation predictions of the pressure and temperature distributions at z=1.25 m are shown in Fig. 3 and Fig. 4. After the ignited by a high explosive charge, a spherical high-pressure region with a shock wave has been formed near the ignition region, where the pressure raises from 0.1 MPa to 1 MPa, as shown in Fig. 3(a). The temperature in this high-pressure region is also up to 2000 K due to the heat release of combustion, as shown in Fig. 4(a). With the development of the shock wave, the structure of shock wave becomes more and more complicated since the shock wave reflects at the top wall, left wall, step and other obstacles, as shown in Fig. 4 (b), (c), (d) and (e). At the same time, the temperature in the combustion region is also increased into 2000 K, as shown in Fig. 5. When the collision between shock waves occurs, the strength of the shock wave is superposed, and the temperature is further increased. The numerical results show that all the complicated shock wave structures could be captured by the TVD numerical Von-Leer scheme without any non-physical oscillation.
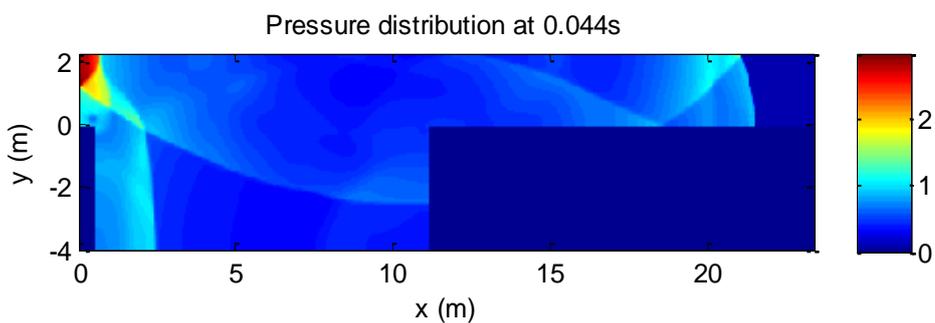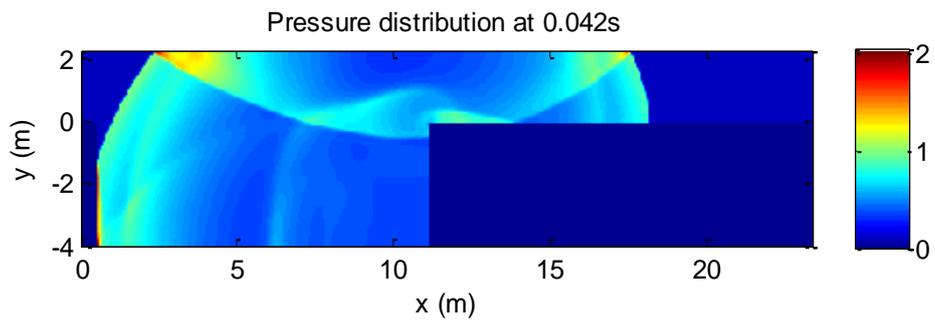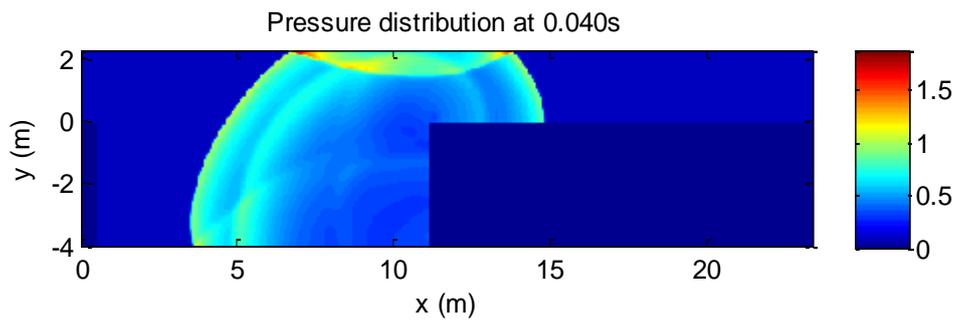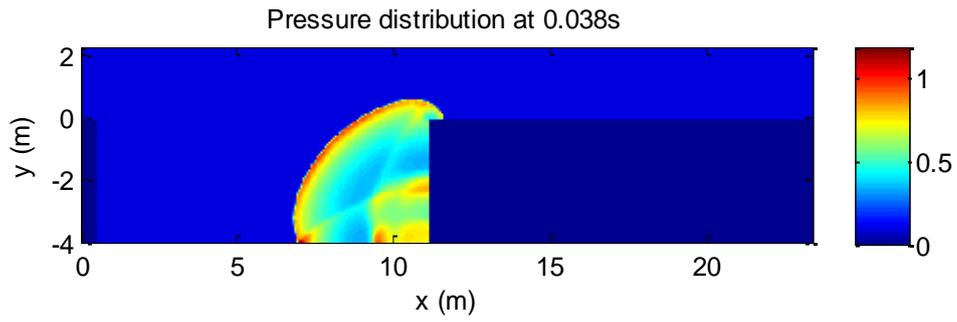

(a)

Pressure distribution at 0.038s

(b)

Pressure distribution at 0.040s
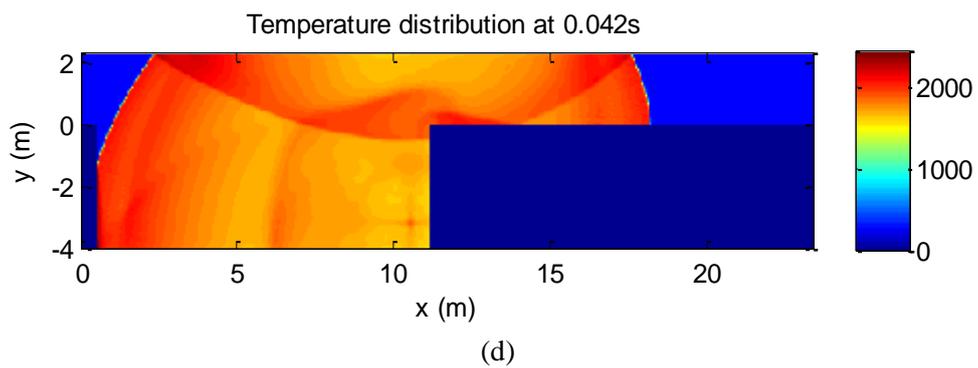
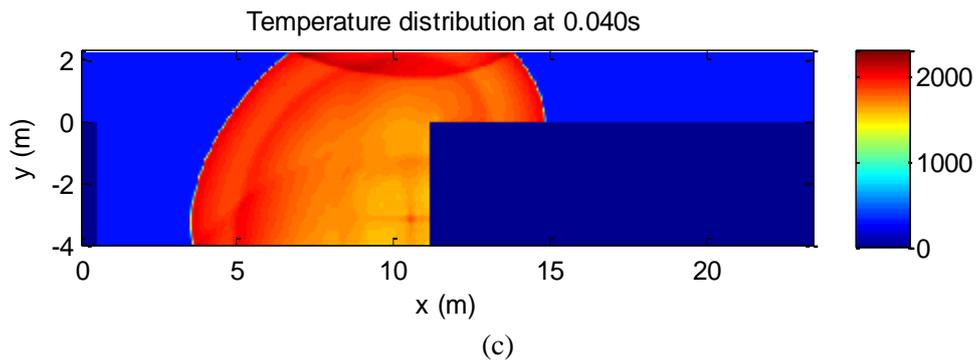(c)

Pressure distribution at 0.042s

(d)

Pressure distribution at 0.044s

(e)

Fig. 3. Pressure distribution at z=1.25 m (MPa)

Temperature distribution at 0.036s

(a)

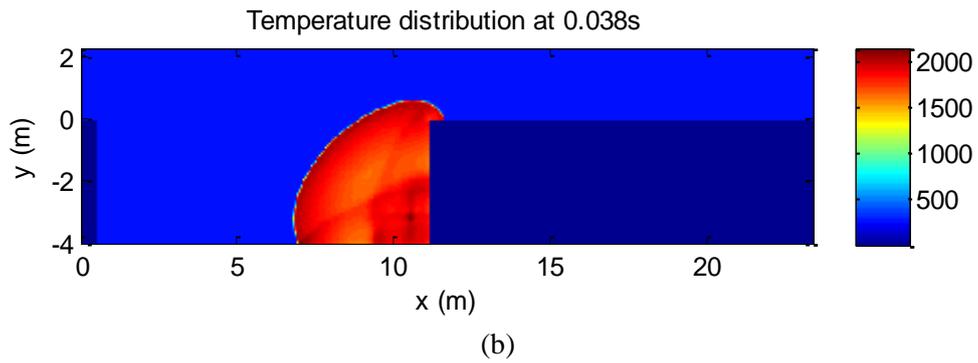Temperature distribution at 0.038s

(b)

Temperature distribution at 0.040s

(c)

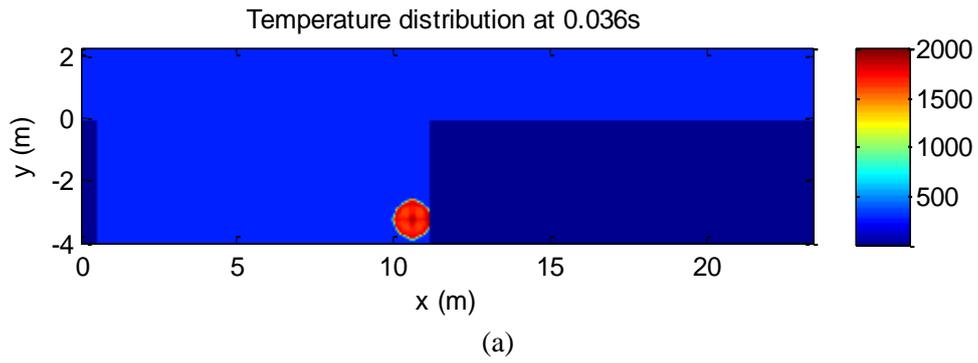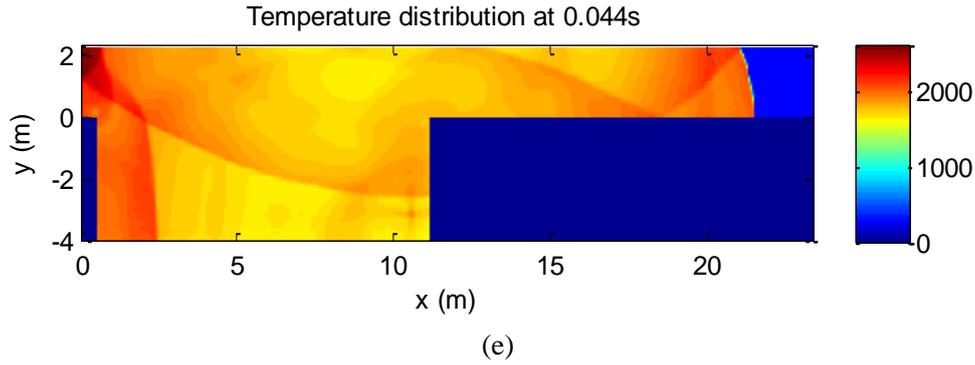Temperature distribution at 0.042s

(d)

5

Fig. 4. Temperature distribution at z=1.25 m (K)

Comparison of the experimental pressure records and the simulated pressure dynamics obtained in 3D simulation are shown in Fig. 5. Pressure transducers 2, 3, 4 and 5, as shown in Fig.2, have been selected for comparison of simulation results and experimental data. The simulated pressure profile for each pressure transducer is in a reasonably good agreement with the experiment if the strong initiation pressure peak is taken into account. In this simulation, the peak value of the pressure is lower than that of the experimental data, since the calculation cell size (5 cm) is coarser than the detonation cell size to reduce the computational cost. The first sensor reached by the explosion (number 2) is taken as a reference. The evolution of the over-pressure signal, the propagation speed and/or the delay of the signals could be compared with the experimental one in different gauges. Joining the first signal peaks as well as later ones (reflections) the propagation of the detonation on the facility could be studied. This is represented in the Fig. 6 as well as the speed of a flat detonation front which resulted to be 1703 m/s. In the interval between the first and the second gauge, the experimental results show an overdriven detonation plus the effect of a curved detonation front (effect of the oblique wall and spherical initial detonation blast). It is represented as the deviation (increase) from the predicted theoretical detonation speed of the planar flame. The rest of gauges, are further away from the initial detonation position. Thus the effect of the initial explosive charge no longer is present. Also the curvature of the detonation front is negligible. Therefore in the two last measurement points, the calculated results show a good agreement with the theoretical values under the expected normal deviation of around 2% (35 m/s).
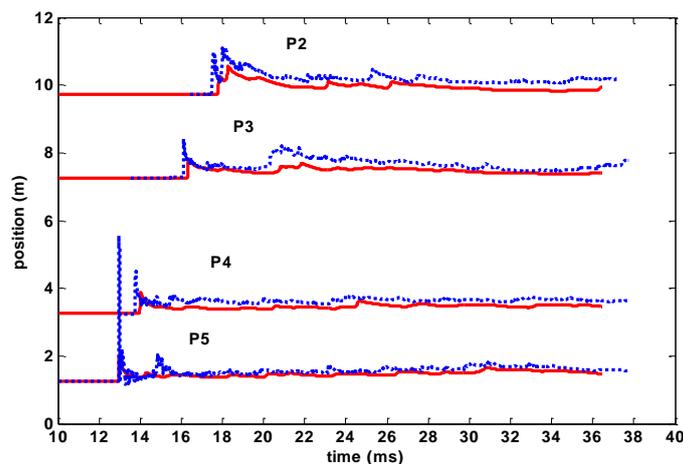

Fig. 5. Pressure history in the canyon along the side wall from the gauges 2 to 5,
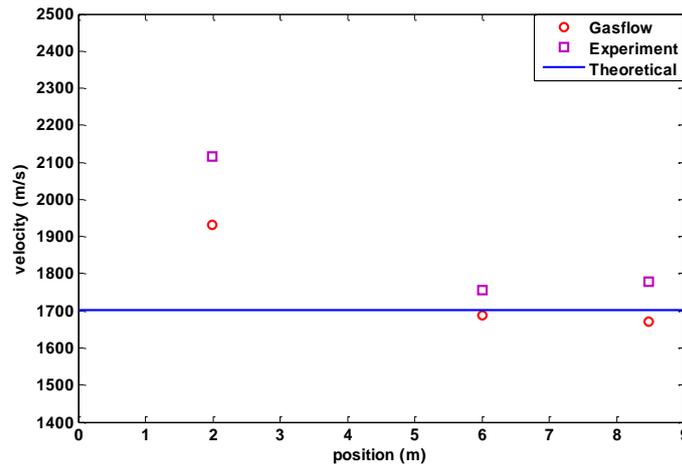(blue dotted line - experiment, red solid line - simulation)

Fig. 6. Detonation speed

4. CONCLUSIONS

GASFLOW-MPI is a well-developed numerical tool to predict the complicated hydrogen behaviors in the three-dimensional large-scale industry facility. For the unintended hydrogen release, the hydrogen-air detonation, leading to huge pressure and thermal load, is viewed as the worst state of affairs. In this work, a numerical study of the detonation benchmark at RUT tunnel facility is conducted to further evaluate the capability of GASFLOW-MPI in simulating the detonation. The numerical results show that the complicated shock wave structures could be captured accurately without any non-physical oscillation by using GASFLOW-MPI. The propagation speeds, overpressures and impulses can be well predicted (deviation of around 2%) using the calculation cell size coarser than the detonation cell size. In general, it can be concluded that the GASFLOW-MPI simulation results of large scale hydrogen detonation in confined geometry are reliable and trustworthy.

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