Detonation in 3D annular chamber with obstacles and water surface on one end

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1 Introduction

Accidents at Hamaoka, the first power nuclear plant, and Fukushima are considered to be due to hydrogen explosion and it was thought that a part of the explosion accidents was caused by detonation. Since the influence of the detonation was not considered by the design of the nuclear power plant, it caused serious damages.

In this study, the relation of flame propagation and obstacles is investigated by calculating parameters such as overpressure and temperature in case of hydrogen explosion in annularly shaped tank with cylindrical obstacles as a representative example. Therefore, in this study, numerical computations are performed. Also the outbreak energy of the explosion to occur in the container, which had a cylindrical obstacles to confirm the safety in the small capacity apparatus that could exist at a nuclear power plant.

2 Background of flame propagation in combustion chamber with cylindrical obstacles

Generally, in the tube which is having obstacles, the surface area of the flame is enhanced by obstacles, and flame propagation speed and the pressure increases. Therefore, it is known that obstacles have an influence on detonation. The propagation mechanism of detonation with obstacles is provided by many researchers, for example by Teodorczyk et al. [1] experimentally and by Shiokawa et al. [2] computationally. It is known that the propagation mechanism strongly depends on blockage ratio, which is the ratio of the height of an obstacle for a pipe diameter. Raise of blockage ratio delivers delays increase at reaction evocation time. In addition, the influence obstacles placement is given by Ogawa et al. [3]. This numerical study showed three stages of flame acceleration and how they are affected by the inclination of the array. At the initial stage, the flame accelerates because of increase in flame surface area by flow around a cylinder. At the inclination

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angle 45°, where the cylinders are staggered, turbulence develops more slowly than at intermediate angles, and this results in the slowest flame acceleration. In the second stage, the flow becomes supersonic, and the shock flame interaction causes the flame acceleration. The final stage is a quasi-steady state of supersonic propagation. The inclination angle has an influence on the position of the local explosion.

3 Numerical method

Because DDT strongly influenced by diffusion, heat conduction and viscosity, the three-dimensional compressible Navier-Stokes equation were used for calculation. Thus, the governing equation is Navier-Stokes equation. Because detonation is a nonsteady phenomenon, explicit method is generally used as integral calculus of the governing equation, but a time step becomes small and calculation cost grows big in the explicit method because it is accompanied by a chemical reaction. Therefore a method called point implicit method is used when detailed chemical reaction is implemented.

4 Detail chemical reaction model

Detonation is caused by rapid chemical reactions, where pressure and temperature suddenly change. Therefore a detailed chemical reaction model expressing a chemical reaction in detail is necessary to solve the issue of detonation. The detailed reaction model is suggested by various researchers including Baulch et al. [4], Petersen et al. [5], Jachimowski [6], Wilson et al. [7], Lefebver et al. [8], Hishida et al. [9]. However, the problem is that it came to have small detonation cell size when a detailed reaction models were indicated for numerical value of fluid analysis. Therefore the importance of 9 chemical species and 18 reactions including pressure dependence built by Petersen and Hanson [5] was shown as a result that Shimizu et al. [10]. However, recently Hong et al. [11] announce the reaction model for hydrogen/oxygen of very high precision. The new mechanism was examined OH and H2O for time-histories in various kinds of H_2/O_2 systems such as H_2 oxidation, H_2O_2 decomposition, and shock-heated H_2O/O_2 mixtures, and it was found that studies agreed very well. In addition, Hong's mechanism is validated against a broader range of more the conventional type of H_2/O_2 movement target such as the flow reactor species of time-histories, the ignition delay times, laminar flame speeds, and a burner-stabilized flame structure. One of the Hong's result is shown in Figure 9. The model of Hong of 9 chemical species was adopted in this study.

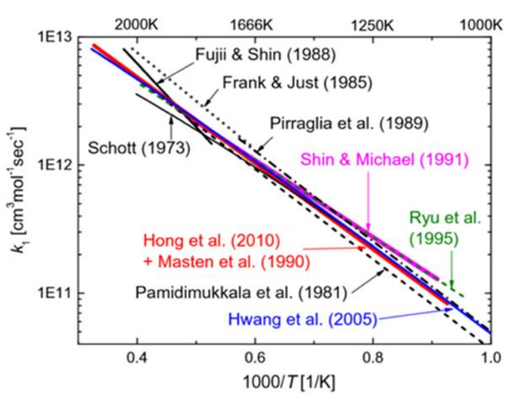

Figure 1. Arrhenius plot for k1 [11]

Table 1: Hong's H2/O2 reaction mechanism. [11]

No.	Reaction	A	n	Ea [cal/mol]	Uncertainty (±%)	T range [K]
1	$H+O_2 = OH + O$	1.04E+14		15,286	10	1100–3370
2	$H+O_2$ (+Ar) = HO_2 (+Ar)[a]	5.59E+13	0.2	0	18–35	1050–1250
	Low-pressure limit	6.81E+18	-1.2	0	–	–
	$H + O_2$ (+H_2O) = HO_2 (+H_2O)[b]	5.59E+13	0.2	0	–	–
	Low-pressure limit	3.70E+19	-1	0	–	–
	$H + O_2$ (+O_2) = HO_2 (+O_2)[a]	5.59E+13	0.2	0	–	–
	Low-pressure limit	5.69E+18	-1.1	0	–	–
	$H + O_2$ (+M) = HO_2 (+M)[a]	5.59E+13	0.2	0	–	–
	Low-pressure limit	2.65E+19	-1.3	0	–	–
	Collider efficiency (N_2 = 1): H_2 = 1.5, Ar = 0, H_2O = 0, O_2 = 0		–	–		
3	H_2O_2 (+M) = 2OH (+M)[c]	8.59E+14		48,560	21	1000–1200
	Low-pressure limit	9.55E+15		42,203	–	–
	Collider efficiency (Ar = 1): N_2 = 1.5, H_2O = 9		–	–		
4	$OH+H_2O_2 = H_2O + HO_2$	1.74E+12		318	27	1020–1460
	$OH + H_2O_2 = H_2O + HO_2$	7.59E+13		7269	–	–
5	$OH+HO_2 = H_2O + O_2$	2.89E+13		-500	27	1600–2200
6	$HO_2 + HO_2 = H_2O_2 + O_2$	1.30E+11		-1603		
	$HO_2 + HO_2 = H_2O_2 + O_2$	4.20E+14		11,980		
7	$H_2O + M = H + OH + M$	6.06E+27	-3.31	120,770		
	Collider efficiency (Ar = 1): H_2O = 0, H_2 = 3, N_2 = 2, O_2 = 1.5					
	$H_2O + H_2O = OH + H + H_2O$	1.00E+26	-2.44	120,160		
8	$OH+OH=H_2O + O$	3.57E+04	2.4	-2111	15–25	1050–2380
9	$O+H_2 = H + OH$	3.82E+12		7948		
	$O + H_2 = H + OH$	8.79E+14		19,170		
10	$H_2 + OH = H_2O + H$	2.17E+08	1.52	3457		
11	$H + HO_2 = OH + OH$	7.08E+13		300		
12	$H + HO_2 = H_2O + O$	1.45E+12		0		
13	$H + HO_2 = H_2 + O_2$	3.66E+06	2.087	-1450		
14	$O + HO_2 = OH + O_2$	1.63E+13		-445		
15	$H_2O_2 + H = HO_2 + H_2$	1.21E+07	2	5200		
16	$H_2O_2 + H = H_2O + OH$	1.02E+13		3577		
17	$H_2O_2 + O = OH + HO_2$	8.43E+11		3970		
18	$H_2 + M = H + H + M$	5.84E+18	-1.1	104,380		
	Collider efficiency (Ar = 1): H_2O = 14.4					
	$H_2 + H_2 = H + H + H_2$	9.03E+14	0	96,070		
	$H_2 + N_2 = H + H + N_2$	4.58E+19	-1.4	104,380		
	$H_2 + O_2 = H + H + O_2$	4.58E+19	-1.4	104,380		
19	$O + O + M = O_2 + M$	6.16E+15	-0.5	0		
	Collider efficiency (N_2 = 1): H_2 = 2.5, H_2O = 12, Ar = 0					
	$O + O + Ar = O_2 + Ar$	1.89E+13	0	-1788		
20	$O + H + M = OH + M$	4.71E+18	-1	0		
	Collider efficiency (N_2 = 1): H_2 = 2.5, H_2O = 12, Ar = 0.75					

The T range [K] corresponds to the published temperature range of the experimental validation for that reaction rate constant. $k = AT^n\exp(E_a/RT)$ in units of [s^{-1}], [$cm^3mol^{-1}s^{-1}$] or [$cm^6mol^{-2}s^{-1}$].

[a] Fcent = 0.7.

[b] Fcent = 0.8.

[c] Fcent = 1.

5 Calculation condition and domain

CRUNCH CFD (Computational Fluid Dynamics) V3.0 by CRAFT Tech Company was used for combustion chamber calculations. CRUNCH CFD is density base CFD Solver by the non-structure lattice limited volume method. For mesh generation Pointwise V17.3 (succession of well-known Gridgen) by Vinas Company was used. Three-dimensional model shown in Figure 2 with cylindrical obstacles in an annular tank was calculated. In this case, outer diameter is "R", inside diameter is "r", height is "h" and diameter of obstacles is "d". Three types of model shown Table 2 were created. One of the models used 350 mm in outer diameter. Grid has 61,956 points and the lattice width is 1 mm. Another model is with outer diameter of 41 mm. The reason why the bigger one couldn't be properly calculated is because of calculation cost. Ignition domain had temperature of 3000 K and the pressure of 0.1 MPa and other case the conditions were 2000 K and 0.5 MPa. Initial conditions were set as in Table 3.

Table 2: Size of model

Case	Dimension	Size of grid [μm]	Grid points	R [mm]	r [mm]	d [mm]	h [mm]
1	**2**	**1000**	**61956**	**350**	**200**	**20**	**-**
2 (4 obstacles)	**3**	**1000**	**217,272**	**41**	**23**	**0.8**	**65**
3 (8 obstacles)	**3**	**1000**	**235,499**	**41**	**23**	**0.8**	**65**

Table 3: Initial condition

Case	⊿t [μs]	Number of iterations	mixture	vol%	T_i [K]	P_i [MPa]
1	**0.025**	**12000**	H_2/O_2	**equivalent ratio 1**	**3000**	**0.1**
2 (4 obstacles)	**0.01 and 0.001**	**41800**	H_2/O_2	**equivalent ratio 1**	**2000**	**0.5**
3 (8 obstacles)	**0.01 and 0.001**	**47900**	H_2/O_2	**equivalent ratio 1**	**2000**	**0.5**

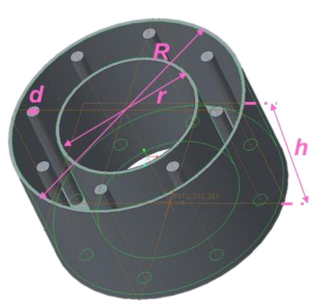

Figure 2. Calculation model

6 Results and summary

Figure 3 shows pressure on slice view. I set points from point 1 to 5 follow this picture. Point 1 is ignition point. Point 2 is maximum velocity point. Point 3 is first point of suddenly rising pressure. Point 4 is leaching outer wall after suddenly rising pressure. And point 5 is flame overlap point.

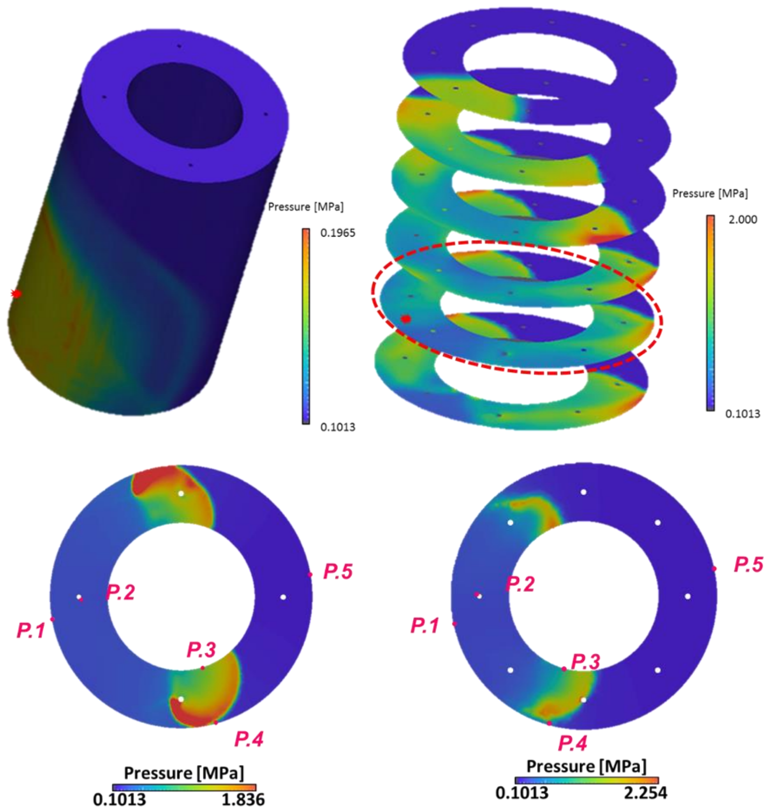

Figure 3. 4 and 8 obstacles on slice view

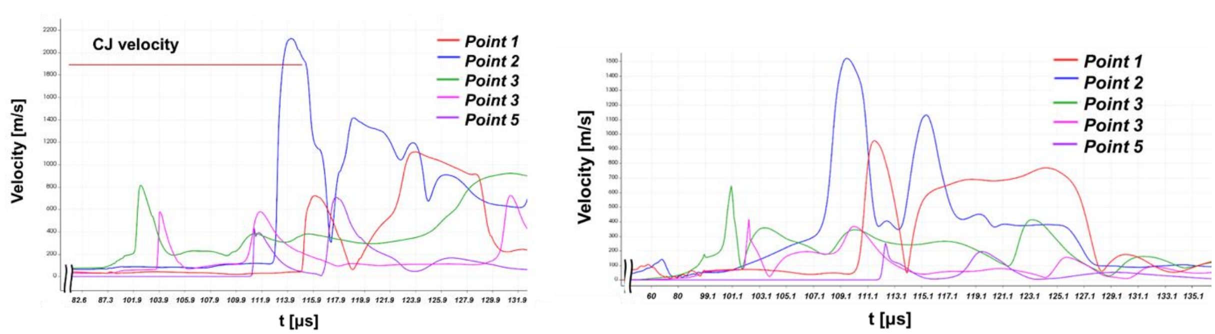

Figure 4. Left: velocity on 4 obstacles; right: velocity on 8 obstacles

Left figure 4 shows velocity property for case A which has 4 obstacles. In this case, Speed is the highest at Point2 and reaches 2,121m/s. This was beyond CJ velocity, detonation was observed. Right figure 4 shows velocity property for case B which has 8 obstacles. In this case, Speed is the highest at Point2 and reaches 1,519m/s. This was not beyond CJ velocity. So detonation was not observed.

Table 4. Comparison 4 and 8 obstacles

	Maximum Pressure [MPa]	**Maximum Temperature [K]**	**Maximum velocity [m/s]**	**Detonation**
4 obstacles	8.234	4,304	2,121	O
8 obstacles	3.868	3,920	1,519	X

4 and 8 obstacles Maximum Pressure is 8.234MPa and 3.868MPa respectively. Maximum Temperature is 4,304K and 3,920K respectively. Maximum velocity is 2,121m/s and 1,519m/s respectively. Detonation occurred only 4obstacles model. Weak detonation occurred with four obstacles. On the other hand, detonation could not be observed with eight obstacles. At the present study shows that was qualitative results are shown, but the distance that reached the peak of pressure and the temperature shortened with obstacles. In addition, the maximum pressure and temperature lowered. Propagation of flame is lowered due to loss of energy when passing obstacles. A future plan is to do a calculation with a model with water placed at the bottom of the chamber. By placing water at the bottom, pressure waves are propagated to water, energy is absorbed, reflected waves are reduced, and it is expected that the peak pressure and temperature will be smaller than when the bottom is a wall.

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