Flame Propagation and Initiation of Detonation in a Two-Dimensional Annular Channel With Cylindrical Obstacles

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1 Introduction

This research investigated combustion scenarios with the aim of eventually developing new safety measures for the prevention of explosive accidents, such as the two serious incidents in Japan at the Fukushima and Hamaoka nuclear power plants. Both events are believed to have involved hydrogen detonations, based on the resulting degree of damage. This study modeled the release of a significant quantity of hydrogen gas followed by an explosion in a two-dimensional annular storage tank in the air-conditioning system of a nuclear reprocessing plant. The objective was to ascertain the effects of obstacles on flame propagation and transition to detonation using numerical calculations. The results obtained with no obstacles and with up to 16 obstacles demonstrate that obstacles render the flame propagation wave approximately 1.2 times slower. However, the presence of obstacles also generates auto-ignition points and shock waves, and the interaction between these shock waves and the propagation wave along the outer wall can contribute energy to the propagation wave. It appears that both auto-ignition and detonation may be more likely when obstacles are present in the channel.

2 Detonation and Deflagration-to-Detonation Transition

Combustion is a rapid oxidation reaction that generates a flame and releases energy. There are two types of combustion: deflagration and detonation. Deflagration is a subsonic combustion in which the rate of flame propagation through the material being combusted is slower than a shock

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wave. In contrast, detonation is an exothermic, supersonic combustion process sustained by a shock wave. During a detonation, premixed gases can be heated essentially instantaneously by a shock wave, and the pressure behind the detonation can increase by a factor of approximately 20. There are two main types of detonation initiations: direct and indirect. Direct detonation is a simple, sudden process caused by a relatively high ignition energy input. In contrast, indirect detonation involves a so-called deflagration-to-detonation transition (DDT). A DDT is a stochastic process triggered by an auto-ignition, a supersonic flame, or an interaction with a shock wave or boundary layer and can be initiated by a comparatively low energy input.

3 Governing Equations

This numerical study used the Navier-Stokes equations below in conjunction with the flux vectors $\boldsymbol{E}$ and $\boldsymbol{F}$ [1].

$$\frac{\partial \boldsymbol{Q}}{\partial \mathrm{t}}+\frac{\partial \boldsymbol{E}}{\partial \mathrm{x}}+\frac{\partial \boldsymbol{F}}{\partial y}=\boldsymbol{S} \tag{1}$$

$$\boldsymbol{Q}=\begin{pmatrix}\rho\\ \rho u\\ \rho v\\ e\\ \rho_1\\ \vdots\\ \rho_N\end{pmatrix},\quad \boldsymbol{E}=\begin{pmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ (e+p)u\\ \rho_1 u\\ \vdots\\ \rho_N u\end{pmatrix},\quad \boldsymbol{F}=\begin{pmatrix}\rho v\\ \rho uv\\ \rho v^2+p\\ (e+p)v\\ \rho_1 v\\ \vdots\\ \rho_N v\end{pmatrix},\quad \boldsymbol{S}=\begin{pmatrix}0\\ 0\\ 0\\ 0\\ \dot{\omega}_1\\ \vdots\\ \dot{\omega}_N\end{pmatrix} \tag{2}$$

4 Grid System

Grid in this study were generated using the Pointwise V17 software by Vinas. Figure 1 and Table 1 present details of the model. The number of obstacles in the channel was varied between 0 and 16 to observe the effects of obstacles. Two grid sizes were used: a coarse grid for 0 and 8 obstacles and a finer one for 16 obstacles. All grids were composed of hexahedrons. Grid sizes are 4 – 40 μm and total number of grid cells is about 2,300,000.

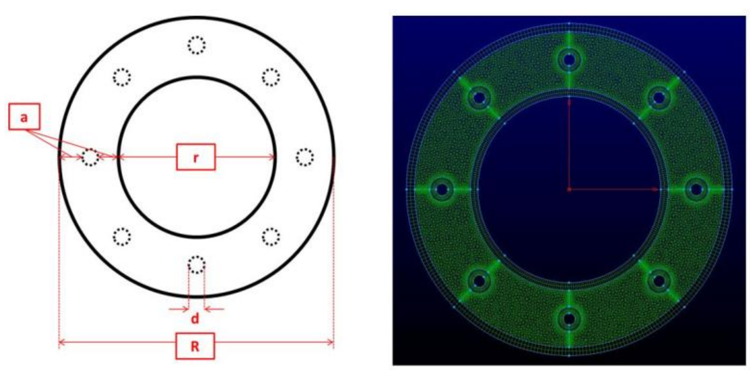

Figure 1. Left: a schematic view of the modeled channel; right: an example of the grid system.

Table 1: Model dimensions (see Figure 1)

Parameter	R	r	D	a
Length [mm]	41	23	1.5	3.25

5 Details of the Chemical Reaction Model

Detonation is caused by rapid chemical reactions, and is associated with exceedingly fast variations in pressure and temperature [2]. Hence, a detailed chemical reaction model is necessary to study detonation phenomena. Hong et al. developed model at Stanford University [3] that allows highly precise predictions for H_2/O_2 systems. This new approach has been used to determine the variations in OH and H_2O concentrations over time in H_2/O_2 systems in different scenarios, including H_2 oxidation, H_2O_2 decomposition, and the shock heating of H_2O/O_2 mixtures, and the results have been found to be in very good agreement with those of previous studies [4, 5]. In addition, Hong's mechanism has been validated against a broad range of conventional H_2/O_2 combustion phenomena, by predicting variations in flow reactor species over time, ignition delay times, laminar flame speeds, and burner-stabilized flame structures. This same model, incorporating nine chemical species, was adopted in the present study.

6 Initial Conditions and Boundary Conditions

The CRUNCH computational fluid dynamics (CFD) software program (V3.0, CRAFT Tech) was employed for all calculations. CRUNCH CFD is a density-based solver that considers equations of state (EOS) as well as compressive and thermodynamic effects. Because this package can calculate only three-dimensional models, the model used in the present work was given a nominal thickness of 1 mm along the z axis. Downside is the restriction to 32 cores only which adds calculation time.

Since this was actually a two-dimensional analysis, the inner and outer walls and obstacle surfaces were modeled as actual, viscous walls (local velocity = 0 at the walls), and the ambient regions were considered to be non-viscous. The entire channel was filled with a stoichiometric mixture (equivalence ratio $\varphi = 1$) of oxyhydrogen, including at the point of ignition on the interior of the outer wall. The ignition point was provided with an ignition energy input in conjunction with high pressure and temperature values. In the case of shock waves (discussed below) the energy inputs from these waves were modeled. The region outside the ignition point (the ambient region) was set to ambient pressure and temperature values.

In the models designated 16 – a, b in Table 2, slightly higher pressure and temperature values were employed in the vicinity of the ignition point to simulate a precursor shock wave that more closely approximated an actual ignition scenario (Table 3).

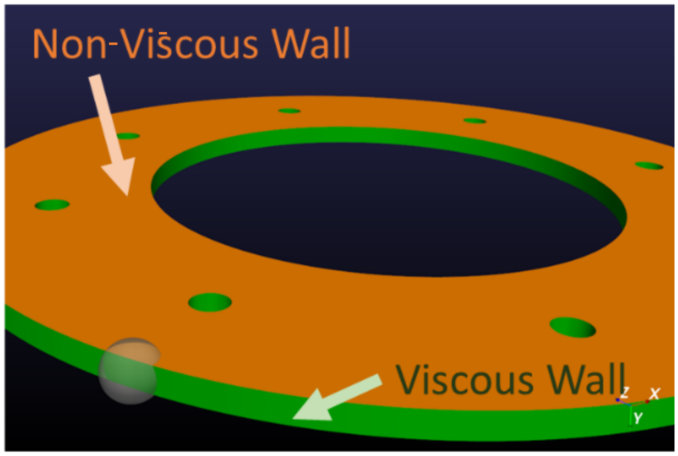

Figure 2 Boundary conditions applied in the model of an annular chamber

Table 2: Initial conditions for calculations

	Ignition Conditions				Grid Conditions		
Obstacles	Radius of the ignition [mm]	Pressure [MPa]	Temperature [K]	Energy [mJ]	Min. Grid Size [μm]	Max. Grid Size [μm]	Number of Grids [10^6]
None	1.5	0.5	2000	130	50	90	2.57
None - a	1.5	0.5	2000	130	10	60	1.30
16	1.5	1.0	2000	260	3.0	40	2.25
16 - a	1.5	1.0	2000	260	3.0	40	2.25
16 - b	1.5	0.5	2000	130	3.0	40	2.25

Table 3: Precursor shock wave conditions at ignition

	Shockwave Conditions			
Obstacles	Radius [mm]	Pressure [MPa]	Temperature [K]	Energy [mJ]
None - a	3.5	0.3	1000	460
16 - a	2	0.5	1000	30
16 - b	3.5	0.3	1000	460

7 Results

Figues 3 and 4 shows pressure and temperature profiles for none and 16 obstacles models. Additionaly Figure.5 compares parameters in time. It can be clearly seen that for the same initial condition and the same mixture initial propagation is faster for none obstacles model. However, one can observe higher energy growth in case of 16 obstacles.

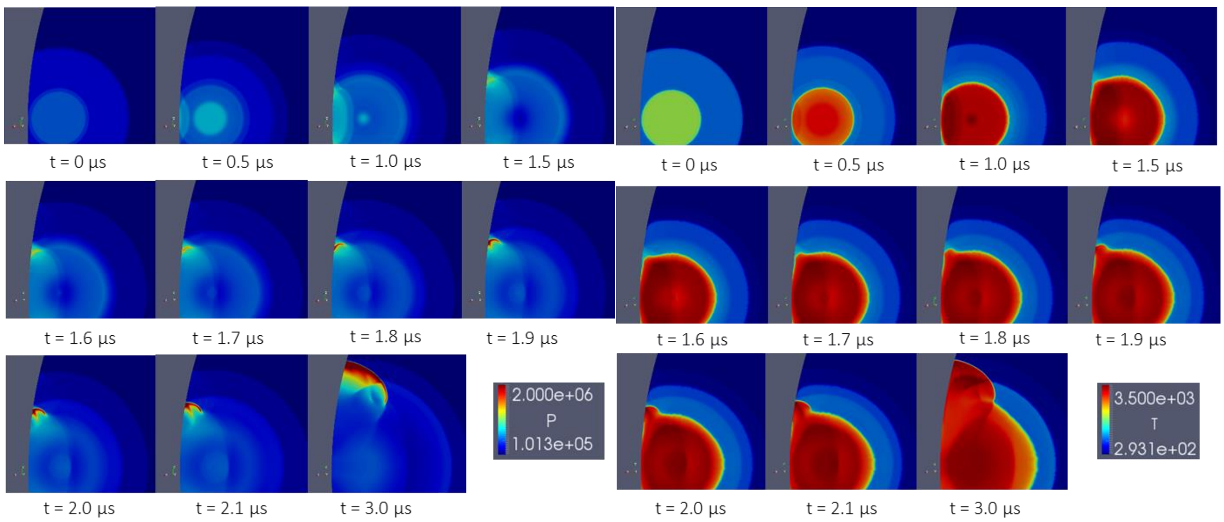

Figure 3 Left: Pressure profiles; right: Temperature profiles. [None - a model]

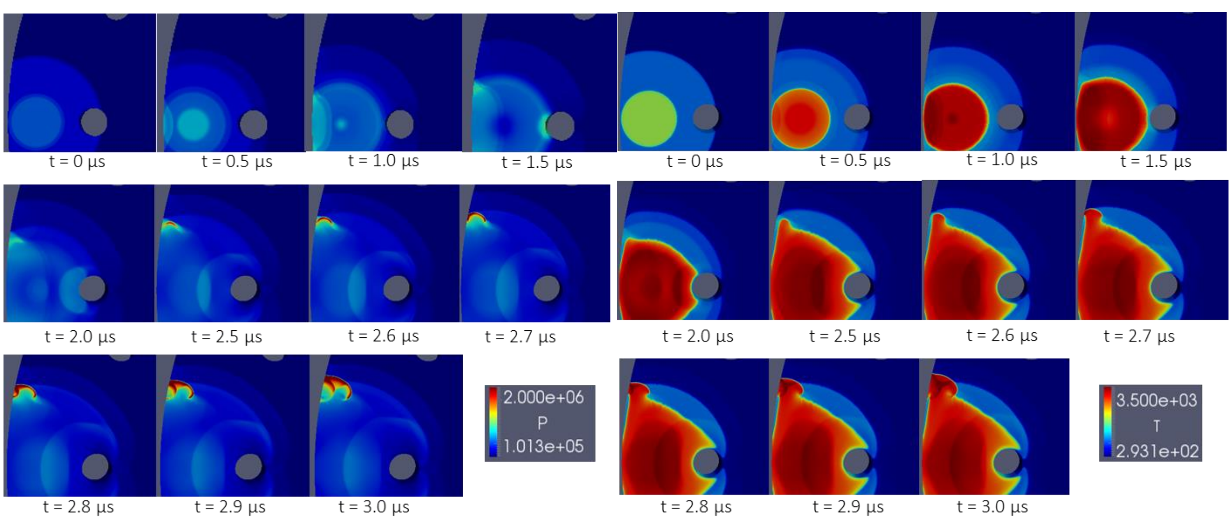

Figure 4 Left: Pressure profiles; right: Temperature profiles. [16 - a model]

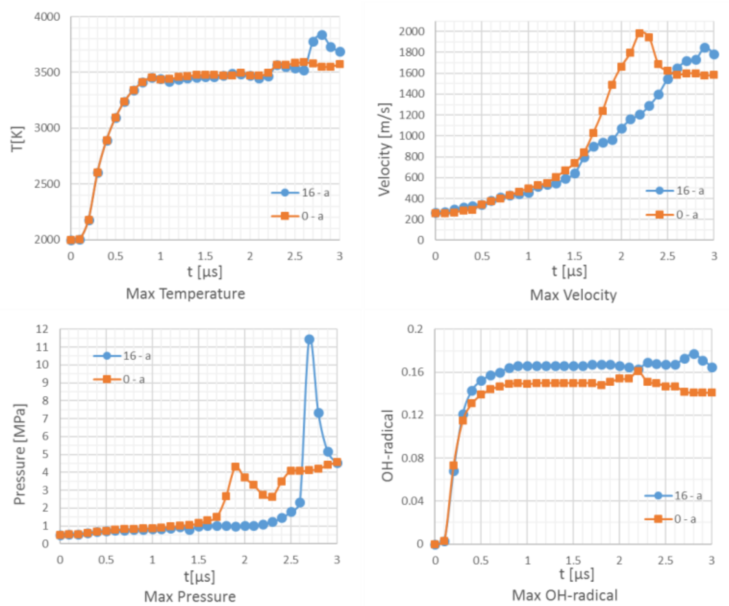

Figure 5 Tables for comparison of [None - a] and [16 - a] model

8 Future work

Results are going to be compared with experiments which are in progress now. Different models are going to employed in the future work. As an example, the layout of the obstacles could be changed so that auto-ignition occurs more often. If ignition takes place solely between obstacles, the resulting shock wave might be reflected by the two obstacles, leading to interactions between waves. Finally, the grid sizes used in the present model were not sufficiently small to precisely mirror actual combustion phenomena. Future models should use finer grids or true three-dimensional grids.

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