

# A Study of the Knocking Mechanism in Terms of Flame Propagation Behavior Based on 3D Numerical Simulations

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## ABSTRACT

The aim of this study is to gain a better understanding of the mechanism of knocking with respect to flame propagation behavior based on 3D simulations conducted with the Universal Coherent Flamelet Model. Flame propagation behavior under the influence of in-cylinder flow was analyzed on the basis of the calculated results and experimental visualizations. Tumble and swirl flows were produced in the cylinder by inserting various baffle plates in the middle of the intake port. A comparison of the measured and calculated flame propagation behavior showed good agreement for various in-cylinder flow conditions. The results indicate that in-cylinder flow conditions vary the flame propagation shape from the initial combustion period and strongly influence the occurrence of knocking.

## INTRODUCTION

In the development process for automotive internal combustion (IC) engines, it is necessary to improve engine performance within a short period of time. This necessity is related to the recent sharp rise in oil prices, rapidly growing awareness of environmental concerns and the shorter life cycles of products today, among other factors. Toward that end, vigorous efforts are being made to utilize numerical simulations in the development of new engines.

Further improvement of the efficiency of internal combustion engines is required today in view of the heightened awareness of environmental issues, including global warming and the depletion of natural

resources, among others. One method that can be cited for increasing engine thermal efficiency is to raise the compression ratio. However, the use of a higher compression ratio is thwarted by the occurrence of knocking. In order to improve the efficiency of internal combustion engines, it is essential to understand the mechanism causing knocking and to take effective measures to prevent it. Extensive experimental work and numerical simulations have been done toward that end. Studies done to explicate the mechanisms present at the time of and following the occurrence of knocking have mainly focused on investigations of knocking intensity.[1-3] With regard to the mechanism that causes knocking, research has principally involved spectroscopic measurements of the end-gas region in visualization experiments[4-6] and investigations of the reaction process based on calculations performed with chemical kinetic simulation models.

In addition to explicating the reaction process prior to the occurrence of knocking and the behavior that subsequently takes place, it is also necessary to have a good understanding of the formation process of the end-gas because that is the region where knocking occurs. In order to analyze the mechanisms involved in this process, it is important to make clear the influence of various factors that affect flame propagation behavior. Three-dimensional combustion simulations provide an effective tool in this regard. For use as a flame propagation model, we have previously developed the Universal Coherent Flamelet Model (UCFM) that can predict the burning velocity under a wide range of engine operating conditions. Using the UCFM, we have developed a 3D combustion simulation for predicting

engine combustion performance, including the occurrence of knocking.[7-8]

The present study focused on flame propagation behavior and the end-gas formation process. Three-dimensional combustion simulations were run to investigate the interaction between in-cylinder flow conditions and flame propagation, something that is difficult to examine experimentally. The results revealed how the in-cylinder flow produced in the intake process and the expansion flow resulting from combustion influence the formation process of the end-gas region where knocking occurs.

## CALCULATION METHODS

The UCFM described above was used in this study as the flame propagation model and the Livengood-Wu integral [10] was used as the model for predicting when autoignition of the end-gas occurs. In order to focus attention on how in-cylinder flow conditions influence the end-gas formation process, the time and place where the value of the Livengood-Wu integral  $c$  reached 1.0 were defined as the time and location of knocking. No calculation was made of heat release due to knocking.

This approach was used to predict the time and location of autoignition of the end-gas. The database of the ignition delay time used in the Livengood-Wu integral was derived with a detailed chemical kinetic model.

The octane number reference fuels of iso-octane and n-heptane were applied in this study as the test fuels, and the simplified mechanism of a blended fuel proposed by Tsurujima [9] was used as the reaction mechanism.

Calculations were performed by incorporating the physical models in Table 1 in the STAR-CD general-purpose computational fluid dynamics (CFD) code. In order to derive the in-cylinder flow and turbulence with good accuracy in the presence of strong swirl, the Renormalization Group (RNG) k- $\epsilon$  model, which generally provides high accuracy for swirl flow, was used as the turbulence model.

Figure 1 shows the calculation grid used in the numerical simulations for comparison and validation with the experimental results. The grid was configured with approximately 400,000 calculation cells at top dead center, including the intake and exhaust ports.

## EXPERIMENTAL VALIDATION PROCEDURE AND ENGINE OPERATING CONDITIONS

A 4-valve single-cylinder test engine with a flat piston and a pentroof combustion chamber was used in the visualization experiments and calculations to investigate the influence of flame behavior on the occurrence of knocking. Table 2 shows the specifications of the test

Table 1 Configuration of 3-D combustion simulation

| Combustion (Flame propagation model) | UCFM [7, 8]                   |
|--------------------------------------|-------------------------------|
| Laminar burning velocity             | Gülder model [11]             |
| Burnt gas dissociation               | Post chemistry model [7]      |
| Wall quench                          | FIST model [12]               |
| Wall heat transfer                   | Extended law of the wall [13] |
| Spark ignition                       | ERC model [14]                |
| Auto-ignition                        | Livengood-Wu integral [10]    |
| Turbulence                           | RNG k- $\epsilon$ model       |

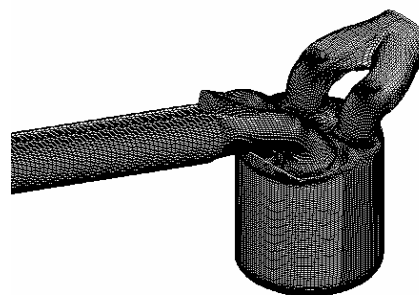


Figure 1 Calculation grid

engine. The fueling method used in the experiments was multi-point injection. In the calculations, it was assumed that the intake gas was a completely homogeneous premixed mixture and the fuel spray in the intake port was not calculated. That was done in order to stabilize the fuel injection quantity regardless of the operating conditions. The residual gas was assumed to be inert and nitrogen was applied as the initial condition in the calculations.

In order to create tumble and swirl flows in the cylinder, the baffle plates shown in Fig. 2 for cases 2 to 4 were positioned in cross section A-A of the intake port. Experiments and calculations were conducted under these flow conditions in the three cases. The tumble and swirl ratios used in each case are shown in Fig. 3.

Table 2 Specifications of test engine

|                    |                                         |
|--------------------|-----------------------------------------|
| Engine Type        | 4-Stroke, 4-Valve, Single Cylinder      |
| Combustion Chamber | Pentroof Type                           |
| Bore x Stroke      | 93 x 81.4 mm                            |
| Displacement       | 552.9 x 10 <sup>-6</sup> m <sup>3</sup> |
| Compression Ratio  | 12:1                                    |
| Fuel               | i-Octane(90%), n-Heptane(10%)           |
| Engine Speed       | 1200 rpm                                |
| Engine Load        | WOT                                     |
| Equivalence Ratio  | 1.0                                     |
| Spark Advance      | -7 deg.ATDC                             |

## VALIDATION RESULTS FOR CALCULATION ACCURACY CONCERNING FLAME PROPAGATION BEHAVIOR

The principal aim of this study was to investigate the influence of flame propagation behavior on knocking by means of 3D combustion simulations. Accordingly, the ability of the simulation model to reproduce flame propagation behavior was validated first. That was done by comparing the calculated results and visualization experiment results regarding the influence on flame propagation behavior of the different in-cylinder flow conditions in case 1 to case 4 indicated in Fig. 2.

Figure 3 shows the in-cylinder flow patterns in the intake process and volumetric efficiencies at all cases. The strong tumble and swirl flows were generated in cases 3 and 4 respectively. Since volume efficiency is almost equal on all the cases, they do not affect the difference in combustion. Finally, experimental tumble and swirl ratios under the all cases are indicated in Figure 4.

Figure 5 compares flame images photographed directly in the visualization experiments with the calculated results for the flame area density  $\Sigma$ . In cases 1 and 2 with relatively weak tumble flow, it is seen that the flame propagates approximately in a concentric pattern centered on the spark plug, with the flame reaching the cylinder wall on both the intake and exhaust sides simultaneously. In contrast, in case 3 with strong tumble flow, the flame reaches the exhaust side earlier. In case 4 with the application of swirl flow, the flame propagates as it turns slowly under the influence of the swirl flow.

In the calculated results, case 3 shows the formation of an end-gas region with negative curvature on the intake side in the latter half of the combustion period and an elliptical pattern of flame propagation is seen in case 4. Thus the simulations were able to reproduce the distinctive flame propagation behavior that occurred from the initial to the later stages of combustion when the in-cylinder flow conditions were changed. Based on these results, it was concluded that the 3D combustion simulation model provides sufficient accuracy for

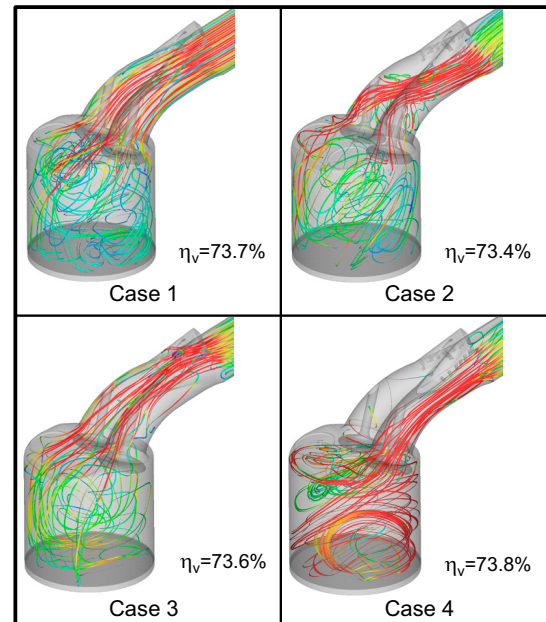


Figure 3 Comparisons of in-cylinder flow pattern and volumetric efficiency

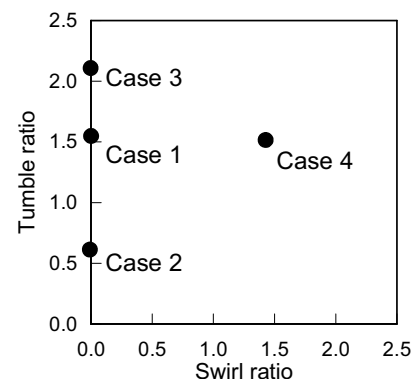


Figure 4 Experimental tumble and swirl ratios under the different conditions as shown in Figure 2

investigating the influence of flame behavior on the occurrence of knocking.

## INVESTIGATION OF MECHANISM CAUSING KNOCKING

Knocking occurs in the end-gas region and knocking intensity is influenced by the quantity and shape of the end-gas at the moment knocking takes place.[5, 15] In order to understand the end-gas formation process better, the calculated results were used to investigate how the in-cylinder flow produced in the intake process and the expansion flow resulting from combustion influence the formation of the end-gas region. The influence of that formation process on the occurrence of knocking was then examined. This section presents the results obtained in this investigation.

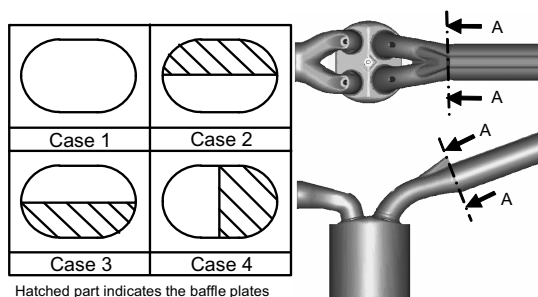


Figure 2 Schematic of baffle plates for producing in-cylinder flow