CFD Solution for HCCI Combustion by Using Parallel Computation and Reduced Mechanisms

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: This study improved the computational efficiency significantly by using parallel computation and reduced mechanisms. To achieve a more accurate analysis, chemical kinetics was implemented into the three-dimensional CFD code, FIRE(tm), to study the intake, spray, ignition, combustion and pollution formation process in HCCI engines. The simulations were run on a cluster of 16-CPU, parallelized using Message-Passing Interface (MPI) mode. The cases with detailed and reduced reaction mechanisms were calculated using 1, 2, 4, 8, 16 CPUs respectively and the corresponding computational time and speed-up were discussed. For the whole HCCI engine simulation, including intake-compression-expansion-exhaust process, the calculation time reduced from 1 month to 1 day using 1-CPU with detailed mechanism and using MPI 8-CPU with reduced mechanism. The solution of using Parallel Computation and Reduced Mechanisms has shown significant reduction in the computational time and fine simulation accuracy. This makes engineering application possible that chemical reaction flow can be applied in ICE combustion simulation to achieve more accurate results.

INTRODUCTION

Homogeneous Charge Compression Ignition (HCCI) has advantages in high thermal efficiency and low emissions and possibly become a promising combustion method in Internal Combustion Engines. Since HCCI is a chemical-controlled combustion process, chemical kinetics must be taken into account for HCCI modeling. However, some investigations have shown that 3D-CFD with detailed chemistry is an illusion. The simultaneous calculation of a detailed fluid mechanics code with a detailed chemical kinetics code is well beyond current computational capabilities [1]. "Current computers can solve the problem of detailed fluid mechanics with very simplified chemistry, or the problem of detailed chemical kinetics with very simplified fluid mechanics, but problem of detailed fluid mechanics linked with detailed chemistry is well beyond the capabilities of even the fast computers." Instead of directly linking fluid mechanics with chemistry, Salvador M. Aceves et. al developed a segregated, sequential multi-zone modeling methodology. In this methodology, running KIVA-3V to obtain temperature profiles which used as input to the followed 10-zone chemical kinetics model. Kong et al [10,11] developed KIVA/CHEMKIN model to simulate the HCCI engine combustion in which the computations started from intake valve closure using a symmetrical 2D mesh of the combustion chamber.

This paper presents a CFD solution of HCCI combustion to resolve the problem of computational capabilities and simulation accuracy using parallel computation and reduced mechanisms

COMPUTATIONAL SETUP

Nowadays, CFD users have realized CPU speed is near to the limitation. Parallel computation is best solution for large scale calculation. However, the computational efficiency of CFD coupled with chemistry is not only dominated by the process quantity, but also relate to parallel mode, mesh scale and reaction mechanism. Therefore, the maximum merit of computational efficiency can be achieved only if these four factors are matched and optimized.

In this study, The simulations were run on a cluster of 16-CPU (all AMD Opteron Processor 280 connected with a 1000 Mbit fast Ethernet, running Redhat Linux AS4.4 64) parallelized using Message-Passing Interface (MPI) mode. The CFD software is AVL FIRE8.42 coupled with chemical kinetics code CHEMKIN 4.9. The compiler is Intel Fortran/C/C++7.1.
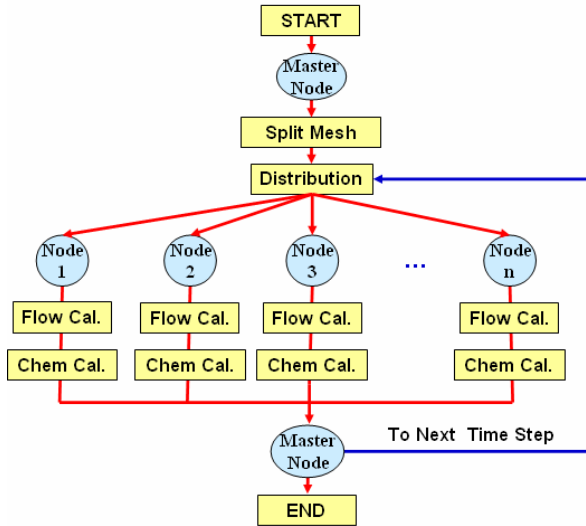

Fig.1　Flow Diagram of Parallel Calculation

Fig.1 shows the flow diagram of parallel calculation using CFD with chemistry. The code starts the calculations with the master node. Then, the computational meshes are split into several parts according the total number of available processors. At the beginning of each time step, the chemistry subroutines for single-zone reactor is called for each computational cell so that the reaction mechanism is taken into account. After the chemistry calculations are completed, the mass fractions of each species are updated as the initialization of flow calculation. After the flow calculations are completed the different processor nodes return their part of the information to the master node. This process is repeated for every time step, as is shown in Fig.1.

HCCI COMBUSTION MODEL

Mathematical Model

1) General Species Transport

General species transport equations, which are solved for an arbitrary number of chemical species, can be expressed as the well-known form:

$$\frac{\partial}{\partial t}(\rho y_k) + \frac{\partial}{\partial x_i}\left(\rho(U_i - U_{\delta i}) y_k\right) = \frac{\partial}{\partial x_i}\left(\Gamma_{y_k}^{ii} \frac{\partial y_k}{\partial x_i}\right) + S_{y_k}$$

where y_k is the mass fraction of the the k-th species.

The mass source, S_{yk}, is defined as:

$$S_{y_k} = \dot{\omega}_k \cdot W_k \cdot V_{cell} \quad ,$$

where V_{cell} is the volume of the computational cell.

2) Energy Conservation Equation

$$\frac{\partial}{\partial t}(\overline{\rho}h) + \frac{\partial}{\partial x_j}(\overline{\rho u}_j\,\overline{h} + \overline{\rho u_j' h'}) - \frac{\partial}{\partial x_j}\left(\frac{\overline{\lambda}}{c_p}\frac{\partial \overline{h}}{\partial x_j}\right) -$$
$$\frac{\partial}{\partial x_j}(\tau_{ij} u_i) - \frac{\partial p}{\partial t} - S_h = 0 \quad ,$$

The energy source, S_h, is calculated by:

$$S_h = \sum_{k=1}^{K} S_k H_k \big|_T \frac{1}{W_k} \quad ,$$

Reaction Mechanism

Four reaction mechanisms of hydrocarbon fuel were adopted in this paper as shown in Tab.1. Iso-octane stands for gasoline-like fuel and n-heptane stands for diesel-like fuel.

Tab1. Reaction mechanisms for HCCI simulation

	Reaction mechanisms	Species	Reactions
1	Detailed iso-octane[3]	89	413
2	Reduced iso-octane[4]	38	69
3	Detailed n-heptane[5]	57	290
4	Reduced n-heptane[6]	42	57

SIMULATION OF HCCI PROCESS

Database of compress ignition characteristics was obtained by measuring cylinder pressure varying with time in RCM (rapid compression machine) filled with hydrocarbon fuels under well-determined conditions in the literature [7]. Fig.2 shows a pressure-time history obtained in the RCM. The rapid compression stroke began with TDC and ends with BDC. After that, the piston was locked. The pressure-time histories were recorded during compression and combustion of the air/fuel mixtures using a Kistler pressure transducer.
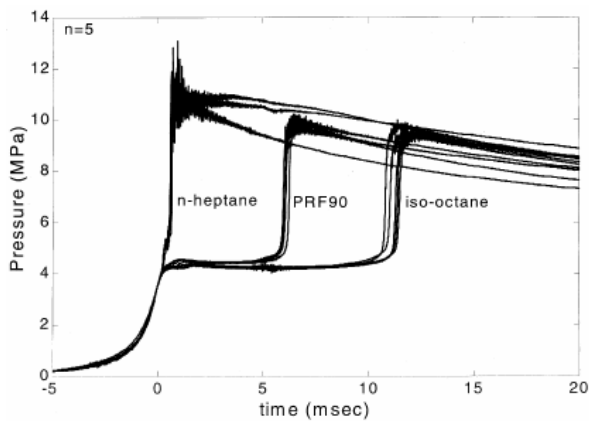

Fig.2 RCM test results with different fuels [7]

（Equivalence raion: 0.4, Initial pressure: 0.1MPa, Initial temperature: 318K, Compression ratio: 16）

However, there is no further investigation on chemical kinetics and flow turbulence. In order to provide a detailed insight into the processes governing combustion and pollutant formation in RCM under HCCI conditions, 3D-CFD coupled with the detailed iso-octane reaction mechanism was used to simulated HCCI process in a rapid compression machine (RCM).

The mains specifications of RCM are listed in Tab.2. The CFD computational grids used for RCM simulation are structured hexahedron mesh. There are 10,200 cells at BDC and 2,000 cells at TDC in the mesh. The moving mesh is generated by FAME ENGINE. In rapid compression stroke, the piston move, so the mesh should move according to a curve of movement description in order to simulate the change of piston position with time.

Tab.2 Specifications of RCM

| Cylinder bore	5.08 cm
Maximum stroke	11.0 cm
Maximum compression ratio	19.0
Clearance height	0.6 — 2.0 cm
Compression time	10 — 30 ms

Fig.4 shows the calculated cylinder pressure curve beginning with 0ms and ending with 30ms. In order to eliminate the effect of combustion, air/co_2 mixture was compressed to obtain pure compression curve as a reference in experiment. While in the calculation, the pure compression curve was obtained by inactivated chemical reactions of air/iso-octane oxidation.

In Fig.4, under inactivated chemical reactions of mixture, global temperature T_c is 832K and cylinder pressure P_c is 4.17MPa respectively at the end of compression, while under active chemical reactions of mixture, T_c is 804K and P_c is 4.03MPa respectively. The two curves deviate at the time of 0.5ms before the compression end. After this deviate point, it clearly can be seen that the pressure value is a little lower than that of pure compression curve until 10.5ms. The start point of first-stage ignition is 0.4ms after the compression end. The start point of second-stage ignition is 10ms after the compression end. Therefore, the ignition delay is 10.5ms. The highest peak pressure after auto-ignition is 9.89MPa, and it is 11.2ms after the compression end.
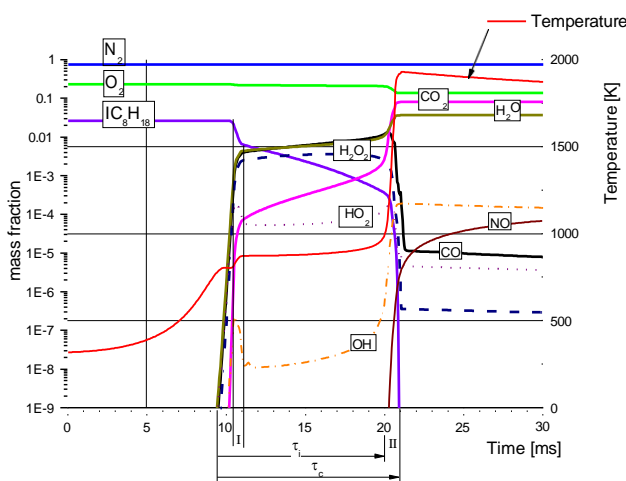
As shown in Figure 2a and 2b, the calculated results including two-stage ignition timings, ignition delay, the peak pressure and dP/dt$_{max}$ agree well with the corresponding experimental results.
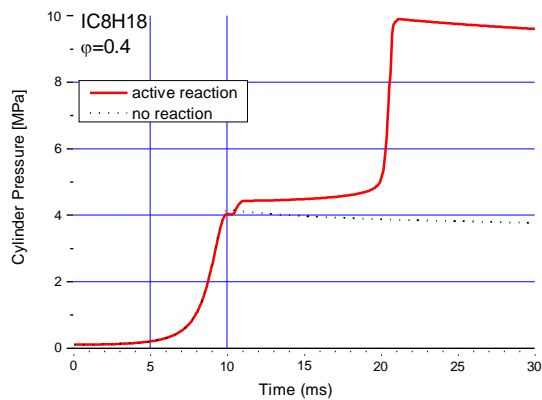
a) Calculated cylinder pressure curve
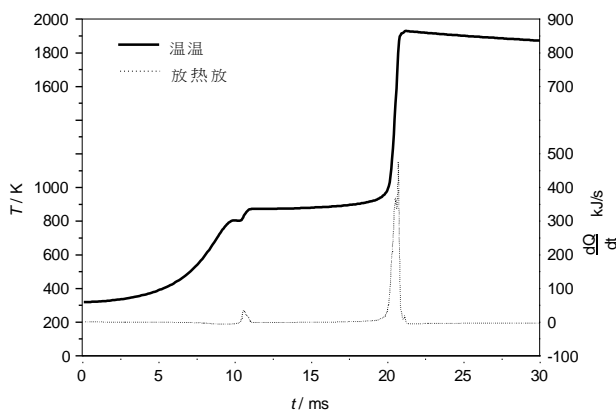
b) Temperature and heat release rate

c) main species history

Fig.3   Calculated two-stage ignition in RCM

(Fuel: iso-octane. Equivalence ratio: 0.4. Initial temperature and pressure: 318 K and 0.1 MPa, respectively. Compression ratio: 16.)

However, the measured in-cylinder pressure decreases faster than the simulated results after the second-stage ignition. It can be explained that the second-stage ignition initiates a branched thermal explosion, which leads to a very rapid pressure rise and a following knocking combustion. While in simulation case, the heat loss is relatively less than in experiment because only normal heat transfer through walls is taken into consideration. It is the possible reason that the cylinder pressure and temperature decrease a little slowly.

Fig.4 shows the concentration of the reactant, product and the global temperature in RCM varying with time. The initial mass fraction of N_2, O_2, IC_8H_{18} is 0.747, 0.227, 0.026 respectively.

As the mixture is compressed, the global temperature rises gradually. Reaction $(C_8H_{18}+O_2=C_8H_{17}+HO_2)$ is initiated by the ion of H from C_8H_{18} by O_2 to form alkyl radical C_8H_{17} and HO_2. Because this reaction is a high endothermic reaction, the temperature begins to be lower than that under inactivated reaction. This is why the deviation between two pressure curves can be observed at 9.5ms mentioned in Figure 2b. At this point, the temperature rises to 780K. Thereafter, the mass fraction of IC_8H_{18} begins to decrease from 0.026.

As compression continues, the temperature rises to 804K at the end of compression stroke. During the intermediate regime, olefin and H_2O_2, are formed gradually. The mass fraction of OH reaches to the first peak at 10.5ms. Then, C_8H_{18} begins to decompose greatly. Meanwhile, the mass fraction of CO increases greatly. Intermediate temperature reaction occurs with small heat release. It leads to a slight temperature rise, so-called the 1st stage ignition (I phase).

After the 1st stage ignition, the temperature in cylinder reaches to 870K. Thereafter, as the temperature increases, the reverse of reaction $(C_8H_{17}+O_2=C_8H_{17}OO)$ is favored and the rate of fuel consumption is decreased. It results in the negative