

Effect of Mesh Structure in the KIVA-4 Code with a Less Mesh Dependent Spray Model for DI Diesel Engine Simulations

Yusuke Imamori, Kenji Hiraoka, Shinsuke Murakami and Hiroyuki Endo

Mitsubishi Heavy Industries, Ltd.

Christopher J. Rutland and Rolf D. Reitz

University of Wisconsin-Madison

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ABSTRACT

Two different types of mesh used for diesel combustion with the KIVA-4 code are compared. One is a well established conventional KIVA-3 type polar mesh. The other is a non-polar mesh with uniform size throughout the piston bowl so as to reduce the number of cells and to improve the quality of the cell shapes around the cylinder axis which can contain many fuel droplets that affect prediction accuracy and the computational time. This mesh is specialized for the KIVA-4 code which employs an unstructured mesh. To prevent dramatic changes in spray penetration caused by the difference in cell size between the two types of mesh, a recently developed spray model which reduces mesh dependency of the droplet behavior has been implemented. For the ignition and combustion models, the Shell model and characteristic time combustion (CTC) model are employed. The calculated spatial distribution of droplets, fuel vapor and soot are compared against high-speed in-cylinder imaging obtained from an optical access diesel engine. Heat release rate, NO_x, soot and computational time are also compared between the two types of mesh. The results show that the uniform-sized mesh reduces computational times significantly while maintaining almost the same prediction accuracy as the KIVA-3 type polar mesh.

INTRODUCTION

Strict requirements in terms of emissions and fuel economy for the off-road diesel engine lead the engine

system to be more complicated. The elements of the engine, for example the air and EGR gas handling parts, the fuel injection system, the turbo-charger etc., must become more flexible to reduce emissions and fuel consumption throughout the operating conditions while maintaining high durability. Engine manufacturers have to understand the combustion process in order to optimize the parameters of these systems in the short term.

Prediction of the combustion process and emissions using a simulation code is useful to reduce the engine development time. Simulations based on the KIVA-3 code are one of the most well-established. Several advanced sub-models has been developed using the KIVA-3 based code. However, it has low mesh flexibility because of employing a structured mesh [1,2,3]. One of the possible problems of the KIVA-3 type mesh is that it is limited only to use a polar mesh when the simulation model applies to a sector to reduce the computational time compared to a full circle mesh. The cell size of a polar mesh varies with location in the radial direction. If a finer mesh is applied in order to improve the resolution around the periphery of the piston bowl, the cell size near the cylinder axis becomes smaller and thinner. Since cells in this region contain a lot of droplets during the injection and combustion events, too small and thin cells lead to long CPU times for the gas phase calculation and can become a possible cause of prediction inaccuracy. The KIVA-4 code which employs an unstructured mesh [4,5] has been released recently and it is thought to be one of the next generation codes because it has the potential to enhance mesh flexibility

while employing almost the same sub-routine structures as the well-established KIVA-3V-release2 code, the newest version of KIVA-3.

On the other hand, the droplet behavior predicted by the standard Lagrangian-Droplet and Eulerian-Fluid (LDEF) based spray model has high mesh-dependency, as reported by various researchers [6,7,8,9]. This means that changing the mesh structure from the conventional KIVA-3 type does not only affect the gas phase but also the droplet behavior. One of the solutions to reduce mesh-dependency is the gas-jet spray model developed by Abani et al. [10,11,12], which is implemented into the KIVA-3V-release2 code.

In this work the gas-jet model is implemented into the KIVA-4 code. Then diesel combustion in an optically accessible single cylinder engine is simulated using the conventional KIVA-3 type mesh and the non-polar mesh with uniform cell size throughout the piston bowl.

SIMULATION CODE

Simulations were performed using the KIVA-4 code. KIVA-4 is an unstructured version of the KIVA code family. Indices of the vertex and cell are perfectly decoupled and a lookup table is used for referring to each other. This is contrasted with the KIVA-3 code which shares the same index between the vertices and cells. Also the cell connectivity in KIVA-4 is independent of these indices. These changes enhance the flexibility of generating grids.

Most sub-models and the flow of the computational process are taken over from the KIVA-3V-release2 code, the latest version of KIVA-3. This eases transferring sub-models from the KIVA-3 based code. Table 1 shows the sub-models of the original KIVA-4 and the current modified KIVA-4 used in this work.

Table 1. KIVA-4 sub-models

Sub-models	Original KIVA-4	Modified KIVA-4
Turbulence	RNG k-ε *	RNG k-ε
Spray	KIVA standard *	Gas-jet
Breakup	TAB *	KH-RT
Collision	O'Rourke *	O'Rourke *
Evaporation	Multi-component	Multi-component
Wall impingement	O'Rourke *	ERC model
Combustion	Eddy Dissipation *	Shell ignition + CTC
NOx	Extended Zeldovich	Extended Zeldovich
Soot	Surovikin + NSC *	Hiroyasu + NSC

* Based on the KIVA-3V-release2 [3]

Figure 1 shows a typical calculation result using the current modified KIVA-4. The result of the KIVA-3V-release2 using the same sub-models is also plotted for comparison. The mesh structure and the cell size in both

cases is same as that named 'Mesh1 (K3-type, base)' described in a later section. Calculation conditions are shown in the section 'experimental setup'. The result shows good agreement between both codes. The CPU time in KIVA-4 is approximately 30% faster than the KIVA-3V-release2 case, as shown in Table 2.

Table 2. Comparison of KIVA-3V-release2-ERC and current modified KIVA-4 CPU times

Code	KIVA-3V-rl2	KIVA-4
CPU time [sec]	7,793	5,332

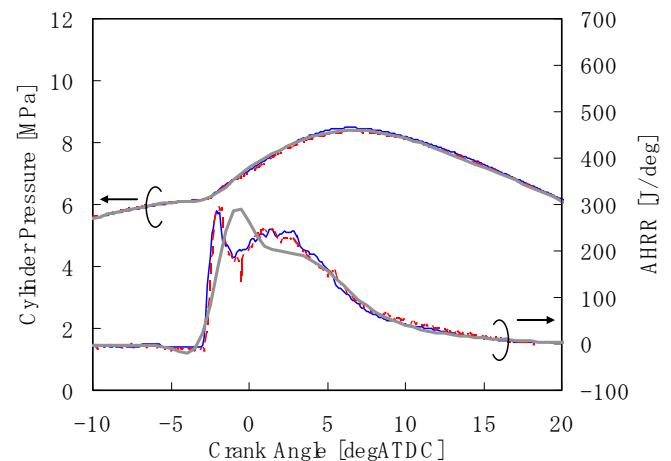


Figure 1. Comparison of KIVA-3V-release2-ERC and the current modified KIVA-4 in cylinder pressure and apparent heat release rate

NUMERICAL MODELING

The spray, droplet breakup, ignition, combustion, NOx and soot models are explained here. Although the droplet impingement model on the wall was also updated from the original KIVA-4, it will not be discussed here because impingement does not occur under the conditions in this work.

SPRAY MODEL

The gas-jet model developed by Abani et al. [10] was implemented into the KIVA-4 code in order to reduce the mesh dependency of the droplet behavior. In this model the relative velocity between the droplet and the surrounding gas in the spray axial direction near the nozzle exit is modeled by gas-jet theory instead of using the gas velocity obtained from the CFD solution directly.

The droplet momentum equation is given as:

$$\frac{dU}{dt} = \frac{3}{8} C_D \frac{\rho_g}{\rho_l} \frac{1}{D} |U - V_{gas}| (U - V_{gas}) \quad (1)$$



Where U is the droplet velocity vector, D is the droplet diameter, V_{gas} is the surrounding gas velocity vector and C_D is the drag coefficient. The perpendicular components to the spray axis of V_{gas} are taken from the CFD solution. V_x , the axial component of V_{gas} , is given by the gas-jet theory [8,13] while x , the axial distance of the droplet from the injector tip, is within two break-up lengths $2L_{BK}$:

$$V_x = V_{\text{gas}} = \min \left[U_{\text{inj}}, \left[\frac{3U_{\text{inj}}^2 d_{\text{eq}}^2}{32\nu_t x \left(1 + \frac{3U_{\text{inj}}^2 d_{\text{eq}}^2 r^2}{256\nu_t^2 x^2} \right)^2} \right] \right] \quad (2)$$

where U_{inj} is the injection velocity of the liquid-jet assumed to be the injection velocity of the gas-jet. r is the radial distance of the droplet from the spray axis. If x exceeds $2L_{BK}$, V_x is assumed to be the velocity $V_{x,\text{CFD}}$ obtained from the CFD solution. The equivalent diameter of the gas jet d_{eq} and the turbulent viscosity for jets ν_t are given respectively as:

$$d_{\text{eq}} = d_{\text{noz}} \sqrt{\frac{\rho_l}{\rho_g}} \quad (3)$$

$$\nu_t = C_t \pi^{0.5} U_{\text{inj}} d_{\text{eq}} / 2 \quad (4)$$

where d_{noz} is the effective nozzle diameter and ρ_l and ρ_g are the liquid and gas-phase densities, respectively. C_t is the entrainment constant. When a revised entrainment constant K equal to $16\pi^{0.5}C_t$ is introduced, Eq. (2) becomes:

$$V_x = \frac{3U_{\text{inj}} d_{\text{eq}}}{Kx \left(1 + \frac{12r^2}{K^2 x^2} \right)^2} ; x \leq 2L_{BK} \quad (5)$$

$$= V_{x,\text{CFD}} ; x > 2L_{BK} \quad (6)$$

Figure 3 shows spray tip penetration in a non-evaporative constant volume chamber calculated by the modified KIVA-4 using the standard KIVA spray model. The cell size is varied from 0.25mm to 4mm. The detailed conditions are described in [10], and the model constants were the same as [10]. Strong dependency of spray penetration on the cell size appears. In the case of the coarse mesh, i.e., 4mm, the penetration is underestimated. The reason for this error is that the cell includes the extra volume in addition to the actual volume that exchanges the momentum with the droplet due to drag forces on the droplet. This leads to under-estimation of the acceleration of the surrounding gas and

results in over-estimation of the drag force on droplets in the following time steps.

Figure 4 shows the result using the gas-jet model under the same conditions as figure 3. The results show independency of the cell size and good agreement with the experiment.

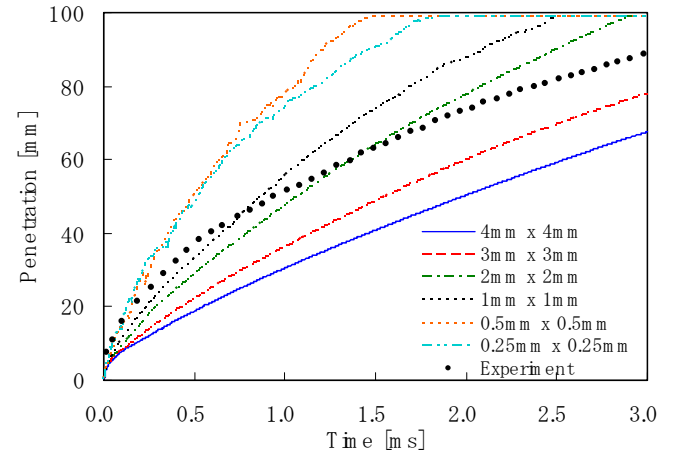


Figure 3. Spray tip penetration in constant volume chamber using standard KIVA spray model calculated by KIVA-4. Cell size is varied from 0.25mm to 4mm. Injection velocity 475m/s, nozzle diameter 257 μ m, gas density 60.6kg/m³.

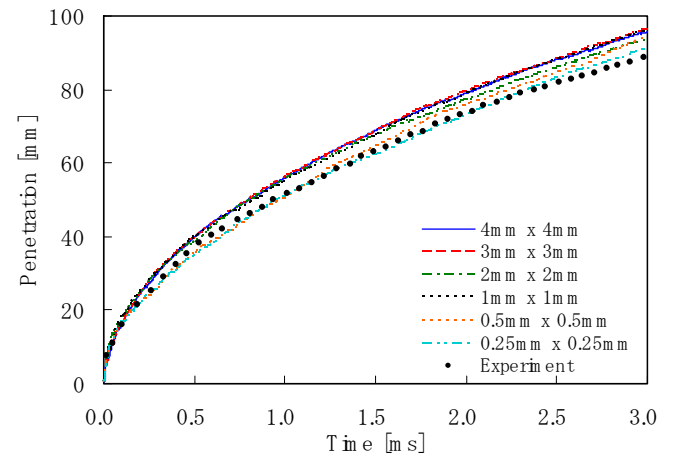


Figure 4. Spray tip penetration in constant volume chamber using gas-jet model calculated by KIVA-4. Cell size is varied from 0.25mm to 4mm. Injection velocity 475m/s, nozzle diameter 257 μ m, gas density 60.6kg/m³.

BREAKUP MODEL

The Kelvin Helmholtz - Rayleigh Taylor (KH-RT) model proposed by Patterson and Reitz [14] was used for the prediction of spray breakup. This model calculates Kelvin-Helmholtz aerodynamic instabilities and Rayleigh-Taylor accelerative instabilities simultaneously. Details of the model can be found in [14]. Model validation was taken from the validation study of a single-cylinder heavy

duty diesel engine using the KIVA-3V-release2 reported by Cantrell et al. [15]. They were kept unchanged throughout all cases, as described in following sections.

IGNITION MODEL

The Shell model proposed by Halstead et al. [16] was employed to predict the auto-ignition process. The chemical mechanism is represented by eight generic reactions and five generic species including fuel, radicals, intermediate species, branching agents and oxidized products. Details of the model can be found in [17]. Since the production reaction of the branching agent is thought to be dominant to determine the ignition timing [17], the pre-exponential constant A_{f4} of this reaction rate was tuned to fit to the experimental data. In the case employing the standard KIVA spray model A_{f4} was set to 5.0×10^5 , and in the case employing the gas-jet model A_{f4} was set to 3.0×10^5 . When the local gas temperature exceeds 1100K, the model is switched to the combustion model described below to simulate the subsequent combustion process.

COMBUSTION MODEL

The characteristic time combustion (CTC) model was used for prediction of the combustion process. This model calculates the equilibrium concentration of each species and the corresponding laminar and turbulent characteristic times to determine species conversion rates. Details of the model can be found in [17]. Although this model is relatively simple, prediction accuracy is sufficient for conventional diesel combustion conditions, such as the case in this work described in the following sections according to detailed comparisons with other advanced combustion models (*i.e.*, the KIVA-CHEMKIN combustion model and the RIF model) using the KIVA-3V-release2 code conducted by Singh et al. [18]. Model constants in this work were taken from [18] and they were kept unchanged throughout all cases described in the following sections.

NOX AND SOOT MODELS

NOx emissions were predicted using the extended Zeldovich mechanism [19], and soot emissions were predicted by a phenomenological 2-step soot model that uses competing formation and oxidation rates. The formation is described by the Hiroyasu soot formation model while the oxidation is predicted by the Nagle-Strickland-Constable (NSC) oxidation model [20]. The parent fuel molecule is used as the species from which the soot forms.

EXPERIMENTAL SETUP

A heavy duty DI diesel engine was simulated in this work. This engine is an optically accessible single-cylinder engine. Table 2 shows the engine and fuel injector specifications. Bottom-view images, which were

observed through a piston-crown window, are used for comparison with the simulations. Detailed description of the engine is available in [21]. Fuel specifications are shown in Table 3.

Table 4 shows the operating conditions. Due to the modification for optical access the compression ratio of this engine was decreased to 11.2:1, so the intake temperature and pressure was adjusted to simulate the in-cylinder condition at TDC of the production engine whose compression ratio was 16:1. The combustion mode in this condition is typical conventional diesel with no-EGR. The ignition delay is relatively short (within 4deg CA).

Table 2. Engine and injector specifications

Engine base type	Cummins N-14
Number of cylinders	1
Combustion chamber	Quiescent
Swirl ratio	0.5
Bore x Stroke [mm]	139.7 x 152.4
Displacement [L]	2.34
Geometric compression ratio	11.2:1
Simulated compression ratio	16:1
Piston bowl diameter [mm]	97.8
Injector type	Common rail
Number of nozzle holes	8
Nozzle orifice diameter [mm]	0.196
Included angle [deg]	152
Nozzle orifice L/D	5

Table 3. Fuel specifications

Cetane number	46
Density @ 20degC [g/cm ³]	0.8426
C/H by weight	6.5
Lower heating value [MJ/kg]	43
Viscosity @ 40degC [cS]	2.35

Fuel type: Phillips Petroleum Ultra-Low Sulfur 2007
Emissions Certification Number 2 Diesel Fuel

Table 4. Engine operation conditions

Speed [rpm]	1,200
IMEP [bar]	4.4
Injection pressure [bar]	1,200
Intake temperature [degC]	111
BDC temperature [degC]	106
Intake pressure [kPa]	233
TDC motored temperature [degC]	905
TDC motored density [kg/cm ³]	24
Peak adiabatic flame temp. [degC]	2,760
SOI [deg ATDC]	-7
Injection quantity [mg]	61
DOI [deg CA]	10
Oxygen concentration [vol%]	21