

Zero-Dimensional Simulation of Diesel Engine Combustion and Emissions Based on CMC Model and Skeletal Reaction Mechanism

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ABSTRACT

A zero-dimensional code is developed to simulate turbulent spray combustion and NO_x and soot emission in direct injection diesel engines. The code consists of two major parts; mixing calculation for the probability density function (PDF) based on the multi-zone model by Hiroyasu et al. (1983) [1] and the flame structure by the conditional moment closure (CMC) model (Klimenko & Bilger, 1999) [2]. The skeletal mechanism of n-heptane is employed with the elementary reaction steps for heat release and the NO_x chemistry in GRI 3.0. The spray model accounts for evaporation and mixing based on momentum balance of the spray zones, while the CMC model incorporates the conditional flame structures with one fuel group or flame structure for each injection. The spatially integrated density-weighted PDF, $F(\eta)$, is defined to represent inhomogeneous mixture distribution in the cylinder. The one-equation soot model is employed for prediction of the soot emission. The program has been validated over a wide range of load and rpm with different injection schedules and EGR levels. Comparison shows reasonable agreement with measurements for the pressure trace and the NO_x and soot emissions for all 16 cases with a single set of tuned constants.

INTRODUCTION

Recently diesel vehicles occupy an increasing market share in Europe and Asia due to their high efficiency and improved electronic control. It has become a critical global issue to develop a new diesel engine with a high efficiency and low emissions to meet ever tightening environmental regulations. Over the years improved injection strategies and charging systems have been implemented to employ a wider range of injection pressures, timings, EGR levels and turbo-charging

and cooling. Computational simulation has proved useful to reduce time and cost for trial-and-error efforts in the development stage of a new engine. Single-zone thermodynamic models have been used extensively as an efficient tool to predict and analyze engine performance. They are based on integral mass and energy balance with some empirical correlations for combustion and other physical submodels [3,4,5]. They cannot resolve turbulent flow field and provides no information on local chemical compositions and temperature in the cylinder. Multi-dimensional CFD codes solve transient 3-D mass, momentum and energy conservation equations to provide local prediction of all averaged vector and scalar quantities. The multidimensional tools have been applied to diverse phenomena including turbulence, combustion, two-phase flow and heat transfer in the cylinder and in other engine components. They usually require quite a few sophisticated submodels and large computational resources, which do not allow easy access for repeated use or prompt response, e. g., in transient cycle simulation. A zero-dimensional multi-zone model may be a promising alternative more realistic and accurate than a single zone model, but not as expensive and difficult to handle as multidimensional codes. They can be applied to multi-cycle transient behaviors with realistic submodels for in-cylinder phenomena such as spray formation, air-fuel mixing, droplet evaporation, ignition and turbulent combustion and pollutant emissions.

The multi-zone model proposed by Hiroyasu et al. [1, 6,7,8,9,10] has been popular and employed by several research groups [11,12,13]. It assumes no interaction among different zones and homogeneous composition in each zone. The fuel-air mixing process is described by momentum balance with experimental correlations for spray penetration and velocity. There were a few recent cycle simulation codes

for integrated system analysis and more realistic combustion simulation. Narayanaswamy and Rutland [14] developed a multi-zone cylinder model which incorporates fuel injection, vaporization, heat transfer and energy/species conservation with detailed chemistry for diesel homogeneous charge compression ignition (HCCI) operation. It was combined with the commercial one-dimensional engine cycle code, GT-Power. In Dulbecco et al. [15] the spray model was composed of the four submodels for evaporation, gas entrainment, turbulence and mixture distribution, which are combined with the detailed tabulated chemistry for diesel HCCI combustion. Inagaki et al. [16] applied the probability density function (PDF) concept to their multi-zone model to consider the effect of spatial inhomogeneities. The in-cylinder region was divided up to five zones. They employed the Shell ignition model and the laminar-turbulence characteristic time combustion model linked to the external cylinder model in GT-Power. Bhawe et al. [17] combined the PDF based stochastic reactor model including detailed chemical kinetics and inhomogeneities in composition and temperature in the cylinder. A quasidimensional multizone combustion code was developed for direct injection diesel engines by Jung and Assanis [13]. It was based on the Hiroyasu's multizone model and experimental correlations for ignition delay and kinetically controlled combustion phase. The rate of mixing controlled combustion was limited by availability of fuel vapor and entrained air in any zone. In this work a new 0-D simulation code is developed to investigate pressure and emissions of a production diesel engine in a wide range of operating conditions including rpm, load, injection schedule and EGR. The Hiroyasu's multi-zone model is also implemented for fuel-air mixing and evaporation which determine the local mixture fraction in each zone and the spatially integrated density-weighted PDF. The CMC model is employed to resolve turbulence-chemistry coupling, while the skeletal n-heptane mechanism combined with the NOx mechanism in GRI 3.0 is applied consistently for ignition, heat release and NOx chemistry.

GOVERNING EQUATIONS

Zero-dimensional simulation is based on the first law of thermodynamics and the mass balance equation. The rate of change of total mass in the control volume is equal to the sum of the mass flow rates into and out of the control volume as

$$\dot{m} = \sum_i (\dot{m}_{i,in} - \dot{m}_{i,out}) \quad (1)$$

where summation is over all open surface elements. The mass flow is the fuel flow only, while intake and exhaust valves are closed from IVC(intake valve closing) to EVO(exhaust valve opening). The fuel fraction, f , is defined as m_f/m , and the rate of change of fuel mass fraction and equivalence ratio are given as

$$\dot{f} = \sum_i \left(\frac{\dot{m}_i}{m} \right) (f_i - f) \quad (2)$$

$$\dot{\phi} = \frac{1}{f_s} \frac{\dot{f}}{(1-f)^2} \quad (3)$$

The first law of thermodynamics can be written for an open system as

$$\frac{d(mu)}{dt} = -P \frac{dV}{dt} + \sum_i \dot{Q}_i + \sum_i h_i \dot{m}_i \quad (4)$$

where u , P and V denote the specific internal energy, pressure and volume. We may get an equation for the rate of change of the temperature after some manipulation and substitution of the ideal gas equation of state in Eq. (4). $\sum \dot{Q}_i$ denotes the total heat transfer which is the sum of convective heat transfer to the cylinder wall and latent heat of vaporization of liquid fuel droplets. Therefore, $\sum \dot{Q}_i$ can be expressed as

$$\sum \dot{Q}_i = \sum h_i A_i (T_i - T) - \dot{Q}_{fg} \quad (5)$$

where T denotes the mean gas temperature. The Hohenberg's correlation [18] is used for the convective heat transfer coefficient. Heat loss due to droplet evaporation, $\sum \dot{Q}_{fg}$, is treated by the Borman and Jhonson [19] model.

DESCRIPTION OF SUBMODELS

MULTI-ZONE MIXING MODEL

The zero dimensional code here consists of two major parts; one is the multi-zone fuel-air mixing model that accounts for inhomogeneous distribution of mixture and the other is the CMC model that accounts for conditional flame structures in turbulent nonpremixed combustion. Each species mass can be obtained from the density-weighted PDF from the mixing model and the conditional species profile from the CMC model. The injected fuel is considered as a continuum within the spray zones near the nozzle exit. The spray is assumed to propagate through the cylinder at a constant velocity until the breakup time. At the breakup time liquid fuel disperses into many small droplets instantaneously and the droplets are decelerated due to the drag by surrounding air. Liquid droplets are heated and evaporated by hot air entrained in each spray zone.

Spray penetration and velocity

Figure 1 illustrates the concept of spray multizones. Each axial zone corresponds to the fuel injected during 0.5 degree

crank angle, while radial zones are divided to have equal fuel mass. The number of axial zones is proportional to the injection duration, while there are ten radial zones for all cases in this study. After impingement on the wall, each zone is further divided into 12 zones in the counterclockwise azimuthal direction to consider motion of the fuel film on the wall.

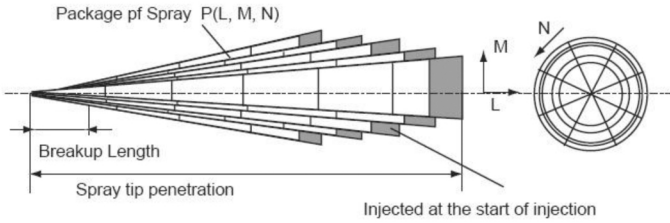


Figure 1. A schematic diagram of the spray zoning model [10]

The initial velocity is estimated from the injection rate profile as

$$V_0 = \frac{\dot{m}}{\rho_l A_{noz}} \quad (6)$$

where ρ_l and A_{noz} denote the density of liquid fuel and nozzle hole area. The spray penetration, S , velocity, V , and breakup time, t_b , of the M -th zone in the radial direction are given as

$$S = 2.95 \left(\frac{\Delta P}{\rho_a} \right)^{0.25} (d_n t)^{0.5} \quad (7)$$

$$V(M) = 1.48 \left(\frac{\Delta P}{\rho_a} \right)^{0.25} d_n^{0.5} [t + t_b(1) - t_b(M)]^{-0.5} \quad (8)$$

$$t_b(M) = 28.65 \frac{\rho_l d_n}{(\rho_a \Delta P)^{0.5}} \exp[-8.557 \times 10^{-3} (M-1)^2] \quad (9)$$

After impingement on the cylinder wall the spray penetration and velocity of the central zone are given as

$$S(1) = K_{imp} t^{0.25} \quad (10)$$

$$V(1) = 0.25 K_{imp} t^{-0.75} \quad (11)$$

$$K_{imp} = \frac{S_{imp}(1)}{[t_{imp}(1)]^{0.25}} \quad (12)$$

The velocity of the M -th zone after impingement is

$$V(M) = 0.25 K_{imp} [t + t_{imp}(1) - t_{imp}(M)]^{-0.75} \quad (13)$$

The following correlation is used to calculate the spray penetration in the swirling gas flow

$$S_s = C_s \cdot S \quad (14)$$

$$C_s = \left(1 + \frac{\pi r_s \text{rpm} S}{30 V_0} \right) \quad (15)$$

where r_s denotes swirl ratio.

Air entrainment

The air entrainment rate is based on momentum conservation of each zone as

$$m_f V_0 = (m_f + m_a) V \quad (16)$$

$$m_a = m_f \left(V_0 / \frac{dS}{dt} - 1 \right) \quad (17)$$

$$\dot{m}_{a,cal} = C \dot{m}_a \quad (18)$$

The air entrainment rate is adjusted by the correction constant C , which is determined independently before and after impingement. The suggested values in Hiroyasu et al. [1] were $C_f=0.7$ before impingement and $C_w=1.5$ after impingement. However, these constants could not reproduce spray mixing in the wide range of EGR rates and split injections for the test engine. Here the two constants are determined to consider different mixing characteristics of multiple injections as

$$C_f = \exp \left[C_1 \frac{m_0}{m_{f,j}} - C_2 t_{inj} \frac{V_0}{d_n} \left(\frac{L-1}{N_{zone}} \right) \right] \quad (19)$$

$$C_w = C_3$$

where L , N_{zone} , m_0 , $m_{f,j}$ and t_{inj} denote respectively the L -th parcel in the axial direction, total number of zones, charge mass trapped in the cylinder at IVC, fuel mass in the j -th injection and injection duration. The term involving C_1 is to consider different mixing rates of multiple injections. It allows easier mixing for an injection with less injected fuel

mass. The term involving C_2 is to consider different mixing rates of multiple zones in a given injection. An earlier injected zone mixes faster with more fresh air than the following zones in any injection.

The spray zones may consume all fresh air under high load conditions according to Eqs. (16) and (17). Interaction among zones is allowed to solve this problem, if there is no more fresh air left for mixing. The air mass entrained from adjacent zones, Δm_a , is given as

$$\Delta m_a = K(m_{a,e} - m_a) \quad (20)$$

$$m_{a,e} = m_{f,z} / (m_{f,t} / m_0) \quad (21)$$

$$K = 1 - \exp[-C_4 \Delta t] \quad (22)$$

where $m_{a,e}$, $m_{f,t}$, $m_{f,z}$ and Δt denote respectively air mass in each zone for the homogeneous mixture state, total fuel mass, fuel mass in a zone and time step. Mixing proceeds to reach the homogeneous mixture state as Δt increases and K becomes equal to unity. Conservation of mass is guaranteed since Δm_a summed up over all zones is always zero. The strategy in Eq. (20) is more efficient than that in Inagaki et al. [16] which should consider mixing between every possible pair of multiple packages with different velocities.

Atomization in each zone is assumed to occur instantaneously at the breakup time. All droplets have the same Sauter mean diameter (SMD), d_{32} given as

$$d_{32} = 23.9(\Delta P)^{-0.135} (\rho_a)^{0.121} (Q)^{0.131} \quad (23)$$

where, ΔP , ρ_a and Q denote effective pressure drop across the nozzle in MPa, air density in kg/m³ and amount of fuel delivery in mm³/stroke [20]. The evaporation rate is calculated by the evaporation model for a single droplet [19] in each zone.

Spatially integrated density-weighted PDF, $F(\eta)$

The spatially integrated density-weighted PDF, $F(\eta)$, is defined as

$$F(\eta) = \int_{V_c} \bar{\rho} \tilde{P}(\eta) dV \quad (24)$$

where $\tilde{P}(\eta)$ is the Favre PDF, which is integrated to be unity in the η -space, [0, 1]. In the 0-D code $F(\eta)$ is obtained by

summing up the mass of the zones whose mixture fraction corresponds to a specific interval in the η -space. $F(\eta)$ describes inhomogeneous distribution of the mixture fraction, which is linked to distribution of all chemical species and temperature through the conditional flame structure.

CONDITIONAL MOMENT CLOSURE MODEL

The conditional mean mass fraction of the i -th species is defined with respect to the mixture fraction, ξ , as

$$Q_i(\eta, t) = \langle Y_i(t) | \xi(t) = \eta \rangle \quad (25)$$

where $\langle \cdot | \cdot \rangle$ denotes conditional averaging for the condition on the right of the vertical bar. A spatially integrated form of the CMC equation in an Incompletely Stirred Reactor (ISR) [21] is

$$\frac{\partial Q_i}{\partial t} = \langle N | \eta \rangle \frac{\partial^2 Q_i}{\partial \eta^2} + \langle w_i | \eta \rangle \quad (26)$$

$$\frac{\partial Q_h}{\partial t} = \langle N | \eta \rangle \frac{\partial^2 Q_h}{\partial \eta^2} + \left\langle \frac{1}{\rho_\eta} \frac{\partial p}{\partial t} \right| \eta \rangle \quad (27)$$

The conditional mean reaction rate in Eq. (26) is modeled in the first order closure as

$$\langle w_i | \eta \rangle \approx w_i(Q_1, \dots, Q_n, Q_h) \quad (28)$$

The conditional mean scalar dissipation rate (CSDR) is modeled by amplitude mapping closure (AMC) [22] as

$$\langle N | \eta \rangle = C_{sdr} \exp(-2[\operatorname{erf}^{-1}(2\eta - 1)]^2) \quad (29)$$

where erf denotes the error function. In the 0-D code the CSDR at the stoichiometric mixture fraction is modeled by

$$\langle N | \eta = \xi_{stoi} \rangle = C_5 \frac{V_0}{d_{noz}} \exp[-C_6 (CA - CA_{sol}) / rpm^{0.4}] \quad (30)$$

where C_5 and C_6 are tuning constants. The constant C_{sdr} is determined to match the stoichiometric CSDR in Eq. (30).

The CMC-ISR model is extended to have multiple flame groups, the number of which is set equal to the number of injections in this work. Hence, $F_j(\eta)$ is defined independently