

Detailed Kinetic Analysis of HCCI Combustion Using a New Multi-Zone Model and CFD Simulations

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ABSTRACT

A new multi-zone model for the simulation of HCCI engine is here presented. The model includes laminar and turbulent diffusion and conduction exchange between the zones and the last improvements on the numerical aspects. Furthermore, a new strategy for the zone discretization is presented, which allows a better description of the near-wall zones. The aim of the work is to provide a fast and reliable model for carrying out chemical analysis with detailed kinetic schemes. A preliminary sensitivity analysis allows to verify that 10 zones are a convenient number for a good compromise between the computational effort and the description accuracy. The multi-zone predictions are then compared with the CFD ones to find the effective turbulence parameters, with the aim to describe the near-wall phenomena, both in a reactive and non-reactive cases. Finally, the model is validated against experimental data of HCCI combustion of fossil and bio-fuels (n-heptane, methyl-hexanoate, and methyl-decanote).

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INTRODUCTION

Homogenous Charge Compression Ignition (HCCI) technology has attracted the attention of the researchers and engineers since more than 30 years. In recent years, the ever increasingly stringent emission standards have lead also the cars manufacturers to see in the HCCI technology the future for the transportation IC engines, due to the promises of improving fuel efficiency and reducing pollutants emissions, with the effect of promoting studies and experiments on it.

Thanks to the auto-ignition mechanism, the system inside an HCCI engine is not characterized by large spatial temperature gradients, like the flame front in spark ignition (SI) engine, with the benefits of reducing NO_x emissions. Furthermore, the premixing of the charge and the very lean conditions allow to reduce soot and particulate matter (PM). However, this combustion system is very difficult to control. Because of the high rates of heat release, that leads to high pressure peaks, and because there is no external devices used to regulate the ignition time (like the spark in SI engine), actually it is still very difficult to guarantee the HCCI

combustion mode along different loads. Moreover, the extremely rapid burning mechanism gives short times to kinetics for completing the combustion reactions, resulting in high emissions of partial combustion products (like CO) [1].

Numerical simulation plays a significant role in the optimization of HCCI combustion and several different models have been presented during the years. It is possible to classify them into two groups. The first one refers to zone models, which focus the interest on the kinetics inside the cylinder, by means of detailed kinetic schemes and a simplified treatment of fluid mechanics and heat transfer phenomena. The second group includes models aimed to study the fluid dynamic and heat transfer processes sacrificing the chemistry, by means of Computational Fluid Dynamics (CFD) tools coupled with reduced kinetic schemes. Since it has been widely demonstrated that HCCI combustion is mainly controlled by chemical kinetics and less affected by fluid mechanics inside the cylinder [2], zone models have acquired great importance in the numerical simulation of such engines.

Zone models follow two main approaches. The first one treats the cylinder volume as a single homogeneous batch reactor with time-variable volume [2, 3, 4, 5]. This “single-zone” model requires a low computational cost but ignores the temperature and composition inhomogeneity inside the cylinder, with the net results of underestimating the combustion duration and overestimating pressure peaks [4]. Moreover, at some extreme conditions, like high Exhaust Gas Recirculation (EGR) and very lean charge, the ignition cannot be correctly predicted [6]. A more sophisticated approach is to improve the single-zone idea and subdivide the cylinder volume into a different number of zones, each of them with its own history of temperature and composition. In this way, the so-called “multi-zone” models allow to take into account charge inhomogeneity. All the versions of the multi-zone model reported in literature mainly differ in the ways that a zone can interact with the neighboring ones. Aceves et al. [7,8] first used a multi-zone model for studying the HCCI combustion and emissions. In this early work, they assumed that the only interaction between zones is due to compression and expansion work. No mass or heat fluxes are allowed. The model was able to reasonably predict the pressure peaks, burn duration and combustion efficiency, but the prediction of CO and unburned hydrocarbons were not completely satisfactory. Mehl et al. [9] developed a multi-zone model on the same concepts, but able to manage detailed kinetic schemes, with a very good prediction of temperature and species profiles inside the cylinder. Another solution is to take into account mass exchange between neighboring zones, as done by Easley et al. [10], Fiveland et. al [11] and Ogink et al. [12], or heat exchanges through conduction [6]. The most complete models take into account interactions through pressure, mass and heat fluxes between neighboring zones, as done by Komninos et al. [13,14] and Kongseereparp et al. [15,16].

Each multi-zone model presented above has the advantage to predict in a good way some relevant aspects of the combustion process inside the cylinder. It is important to observe that some simplifications and assumptions are required to manage the modeling of this complex system in a reasonable time. The purpose of this paper is to present a predictive multi-zone model able to predict the combustion process of an HCCI engine and the pollutant emissions under a wide range of operating conditions and with different bio and traditional fuels. The focus is on the kinetics of the system, with the aim to perform detailed kinetic analysis, like rate of production and sensitivity analysis, since the identification of the paths leading to pollutant formation allows to suggest new engine configuration or operative conditions to strongly reduce the emissions.

The structure of this paper is the following. First, the assumptions on which the model is based are here presented, followed by its description. After this, the CFD activity used for the tuning of the multi-zone model is described. Finally, validation activity is presented, by means of a comparison with experimental data.

CHEMICAL KINETICS

The kinetic modeling of the autoignition of hydrocarbon fuels in HCCI engines requires a careful analysis of both low and high-temperature mechanisms. A general detailed kinetic scheme, consisting of more than 430 species and 13500 reactions, was discussed in previous papers [17,18]. This model, widely validated in both high and low temperature conditions, was recently extended to bio-fuels, such as alcohols and methyl-esters [19, 20, 21]. A brief summary of the fundamental aspects of the mechanism is here presented.

The overall combustion scheme is based on a detailed core mechanism of C1-C4-species and permits description of the oxidation of hydrocarbons up to jet fuels and diesel [22]. The mechanism uses a lumped description of the primary propagation reactions of larger species and primary intermediates. This approach, together with an extensive use of structural analogies and similarities within the different reaction classes, easily allows extension of the scheme to new species [23]. The thermodynamic properties are taken from different thermodynamic databases [24,25] or evaluated on the basis of Benson additivity rules [26].

This kinetic mechanism has been validated in a wide range of operating conditions through the comparison with experimental measurements carried out in well controlled reaction environments (jet stirred reactors, rapid compression machines, shock tubes, flow reactors, ...) [27,28]. The comprehensive validation proved the reliability of the mechanism in all the conditions relevant to engine combustion, extending the possible fields of investigation far beyond the conditions here discussed. The same kinetic scheme, which is capable of simulating the combustion behavior of real transportation fuels [22], has been also successfully applied to the evaluation of the auto-ignition propensities of different fuel surrogate components and mixtures in SI and HCCI engine over a wide set of operating condition, as discussed in previous works [29, 30, 31, 32]. All the quoted results are obtained using the kinetic scheme POLIMI_TOT1212, available in CHEMKIN format with thermo and transport data at [33].

MULTI-ZONE MODEL

The model presented in this paper is a further evolution of the one developed by Mehl et al. [9] for a four stroke single cylinder engine. Since the focus is on the combustion phase, only compression and expansion are described during a simulation cycle. The effects of complex fluid dynamics phenomena such as flows through valves and other dynamic effects are neglected, as well as valve overlapping. The model takes into account the effect of the internal EGR, therefore it is necessary to simulate several cycles to obtain a stability on the cylinder composition. The cycle starts at Intake Valve Closing (IVC) and the cylinder volume filled with the air-fuel mixture. The compression phase occurs until a transition point where chemical reactions become important. During all the simulation, the model accounts for

the chemical phenomena, heat and mass transfers, and it works both in single and multi-zone configurations. Once the expansion phase is completed, a sub-model allows to evaluate the characteristics of the EGR and a new cycle starts. The initial charge composition of the new cycle is evaluated assuming a complete mixing of the EGR evaluated above and the fresh charge, without overcoming the constrain derived from the available cylinder volume. Neighboring zones can interact through work, heat and mass diffusion at interfaces. Convective fluxes are not described. All the contributions considered are both laminar and turbulent.

MODEL EQUATIONS

The mathematical formulation of the model derives from different assumptions. The first one is that the mixture inside the cylinder is modeled as an ideal gas. We also assume that pressure inside the cylinder is uniform. The discretization of the reactive volume is based on the space, and provides for the division into a user-defined number of zones, each one considered as an ideal batch reactor with time-variable volume and uniform temperature and composition. Crevices are not described. During all the simulations presented in this work, the initial temperature and composition of the zones are the same, but it is also possible to specify a distribution for both variables. Throughout the cycle each zone follows its own dynamic, by means of heat and mass diffusion, including the enthalpy effects associated to mass diffusion. The outer zone, representing the boundary layer, is also involved in the thermal exchange with the cylinder and piston walls.

Zone Configuration

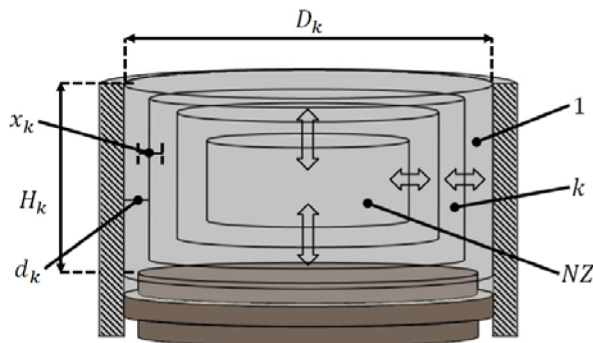


Figure 1. Qualitative topology of the zones used in the model.

Figure 1 shows the topology of the zones. The division of the reactive volume is based on cylindrical zones with an increasing thickness going from the outmost to the inner zone. This solution allows to overcome a typical problem of multizone models, which is the definition of the dimension of the boundary layer. As well known in the literature [7,8], the introduction of a boundary layer allows to better describe temperature gradients of the near-wall region of the combustion chamber. Its dimension is usually defined directly by the user (in terms of volume or mass percentage)

[7,8] or indirectly derived from the number of zones [13,14]. However, the model results are very sensitive to the definition of the boundary layer dimension, especially the correct prediction of the ignition phenomena. The solution proposed in this work allow to refine the discretization in the near-wall region where the significant temperature and composition gradient are present. The idea is to adopt a “mesh” refinement, similarly to what usually done in CFD simulations. At the beginning of each cycle, the cylinder volume is subdivided into zones, each one proportional to a weight w_k :

$$w_k = \frac{1}{(NZ - k + 1)^a} \quad (1)$$

a is user-defined constant that in this work is assumed equal to 1.5. These weights are then renormalized. An example of values of these weights for a 10 zone configuration is reported in Table 1.

Table 1. value for the zone weights calculated using equation (1) and 10 zones.

Zone Index	w_k
1	0.0158
2	0.0186
3	0.0221
4	0.0271
5	0.0341
6	0.0448
7	0.0626
8	0.0964
9	0.1772
10	0.5012

Zone 10 corresponds to the inner one, while zone 1 is the closest to the cylinder walls. Once the zone volumes are known, all other information about zone geometry can be derived by means of simple geometrical constrains. For each zone the ratio:

$$\frac{D_k}{H_k} = \frac{D_{cyl}}{H_{cyl}} = \beta \quad (2)$$

varies according to the crank angle and the compression ratio. In this way β is the same for all zones and the relative shape of the zones resembles that of the total cylinder volume. The diameters and the heights can be calculated as:

$$\begin{cases} D_1 = \sqrt[3]{\frac{4\beta V_{cyl}}{\pi}} \\ D_k = \sqrt[3]{\frac{4\beta(V_{cyl} - \sum_{j=1}^{k-1} V_j)}{\pi}} \quad k = 2, \dots, NZ \end{cases} \quad (3)$$

During the cycle the volume of the zones varies due to the piston movement.

The total volume available for combustion in the cylinder is calculated using the model suggested [34]:

$$\frac{d(V_{cyl}/V_{clear})}{dt} = \frac{d\theta}{dt} \left(\frac{CR-1}{2} \right) \times \sin \theta \left[1 + \frac{\cos \theta}{\sqrt{Z^2 - \sin^2 \theta}} \right] \quad (4)$$

where Z is the ratio between the connecting rod length L_C and the crank-arm radius L_A :

$$Z = \frac{L_C}{L_A} \quad (5)$$

Species Conservation

As already discussed, each zone is considered as an ideal batch reactor with uniform composition, variable volume and open to mass and heat exchanges. Then, the conservation equation in terms of mass fractions ω for each species i in the zone k is:

$$\begin{cases} m_{tot}^1 \frac{d\omega_i^1}{dt} = -A^1 J_i^1 + \Omega_i^1 MW_i V^1 \\ m_{tot}^k \frac{d\omega_i^k}{dt} = A^{k-1} J_i^{k-1} - A^k J_i^k + \Omega_i^k MW_i V^k \quad k = 2, \dots, NZ \end{cases} \quad (6)$$

J_i^{k-1} and J_i^k represent the inlet and outlet diffusive fluxes of the zone respectively. Each J is considered as the sum of the laminar and turbulent contributions:

$$J_i^k = J_{L,i}^k + J_{T,i}^k \quad (7)$$

Following the Fick's law, the laminar flux can be rewritten as:

$$J_{L,i}^k = \rho^k \mathcal{D}_{L,i}^k \nabla \omega_i^k \cong \rho^k \mathcal{D}_{L,i}^k \frac{(\omega_i^{k-1} - \omega_i^k)}{x^k} \quad (8)$$

The laminar diffusion coefficient $\mathcal{D}_{L,i}^k$ is evaluated in each zone and at each time step [35,36]. x^k is defined in Figure 1.

The turbulent flux is defined as:

$$J_{T,i}^k = \mathcal{D}_{T,i}^k \frac{(\omega_i^{k-1} - \omega_i^k)}{x^k} \quad (9)$$

The turbulent diffusion coefficient is evaluated on the basis of fluid dynamic considerations, as described in the next sections.

Energy Conservation

According to the assumptions listed above, the conservation of energy for each zone k is:

$$\begin{cases} \frac{dU^1}{dt} = \dot{Q}_{ext} - \dot{Q}^1 + \dot{W}^1 \\ \frac{dU^k}{dt} = \dot{Q}^{k-1} - \dot{Q}^k + \dot{W}^k \quad k = 2, \dots, NZ \end{cases} \quad (10)$$

The left term of the equation (10) can be rewritten introducing the equation (6):

$$\begin{aligned} \frac{dU^k}{dt} &= \frac{d(\sum_{i=1}^{NS} m_i \tilde{u}_i)^k}{dt} \\ &= m_{tot}^k \langle \tilde{C}_v^k \rangle \frac{dT^k}{dt} \\ &+ \sum_{i=1}^{NS} \tilde{u}_i^k (A^{k-1} J_i^{k-1} - A^k J_i^k) \\ &+ V^k \sum_{i=1}^{NS} \tilde{u}_i^k \Omega_i^k MW_i \end{aligned} \quad (11)$$

The conductive fluxes take into account the heat exchanged between neighboring zones. Starting from the Fourier's law, these terms are calculated with the same approach used for the diffusive fluxes and the diffusion coefficients:

$$\dot{Q}^k = A^k \lambda_{tot}^k \nabla T^k = A^k (\lambda_L^k + \lambda_T^k) \frac{(T^{k-1} - T^k)}{x^k} \quad (12)$$

The term $\dot{W}^k$ in equation (10) contains only the effects of pressure on the zone volume:

$$\dot{W}^k = -P \frac{dV^k}{dt} \quad (13)$$

The heat loss with the cylinder wall $\dot{Q}_{ext}$ is a non-zero term only for the outmost zone:

$$\dot{Q}_{ext}^1 = Ah(T_w - T^1) \quad (14)$$

where h is the exchange coefficient between the zone and the cylinder wall, that it is supposed to be at T_w .

The heat transfer coefficient h is calculated according to the model proposed by Woschni [37]:

$$Nu = a Re^b \quad (15)$$



The constant value used are $a = 0.035$ and $b = 0.8$. For a better description of the heat exchange phenomena, the Reynolds number is evaluated taking into account the effect of the mean gas velocity inside the cylinder $\langle v \rangle$ instead of the mean piston one:

$$\langle v \rangle = C_1 \langle S_p \rangle + C_2 \frac{V_{cyl} T^0}{P^0 V^0} (P - P_{motored}) \quad (16)$$

C_1 and C_2 are two different constants that are assumed equal to 2.28 and 0.324 respectively. $\langle S_p \rangle$ is the mean piston speed defined as:

$$\langle S_p \rangle = 2L_A \varphi \quad (17)$$

$P_{motored}$ is the pressure associated to an isentropic compression between the beginning of the cycle and the actual state:

$$\frac{P_{motored}}{P^0} = \left(\frac{V}{V^0} \right)^{c_p/c_v} \quad (18)$$

The final form of the energy balance is:

$$\begin{aligned} m_{tot}^k \langle \tilde{C}_v^k \rangle \frac{dT^k}{dt} = & \sum_{i=1}^{NS} \tilde{u}_i^k (A^k J_i^k - A^{k-1} J_i^{k-1}) \\ & - V^k \sum_{i=1}^{NS} \tilde{u}_i^k \Omega_i^k MW_i - P \frac{dV^k}{dt} \\ & + Ah(T_w - T^k) + \dot{Q}^{k-1} - \dot{Q}^k \end{aligned} \quad (19)$$

Turbulence Model

The coefficients requested for evaluating the turbulent fluxes of heat and mass can be obtained through the introduction of the turbulent viscosity μ_T [38]:

$$\mathcal{D}_T^k = \frac{\mu_T^k}{Sc_T} \quad (20)$$

$$\lambda_T^k = \frac{Cp^k \mu_T^k}{Pr_T} \quad (21)$$

where Sc_T and Pr_T are respectively the Schmidt and Prandtl number, that for a turbulent flux are assumed equal to 0.7 and 0.85. The turbulence viscosity can be calculated from the turbulent kinetic energy K and the energy dissipation rate ε :

$$\begin{cases} \mu_T^1 = 0 \\ \mu_T^k = \frac{0.09 \rho^k K^2}{\varepsilon} \end{cases} \quad k = 2, \dots, NZ \quad (22)$$

$$K = \frac{3}{2} (u')^2 \quad (23)$$

$$\varepsilon = C_\mu^{3/4} \frac{K^{3/2}}{L_I} \quad (24)$$

C_μ is a constant equal to 0.09 [38], while L_I is the integral length scale and u' the turbulent velocity fluctuation. These two last parameters are estimated from CFD simulations as discussed in the following. μ_T^1 is equal to zero because it refers to the cylinder wall.

Internal Exhaust Gas Recirculation

The exhaust gas that remains trapped inside the cylinder between two cycles plays an important role on the combustion inside HCCI engines. These exhaust gases contain hot species deriving from the partial or complete combustion, like CO and CO₂, that can modify the kinetics of the system when mixed with the fresh charge at the beginning of a new cycle [39]. In the code a simple sub-model is implemented for evaluating the exhaust gases temperature and composition, since the discharge and aspiration phases are not described.

During the exhaust phase, the piston moves from BDC to TDC while the exhaust valve is open. In this process, the exhaust gases exchange heat with the cylinder wall, while the pressure moves from the value reached at BDC to the one of the exhaust pipe. By simplifying this dynamic, we can assume that:

$$\begin{cases} P_{BDC}^{EGR} = P_{end\ cycle} \\ P_{TDC}^{EGR} = P_{atmospheric} \end{cases} \quad (25)$$

During this process, the EGR temperature decreases because of the expansion. The final temperature of EGR at TDC is obtained by assuming that the expansion can be described through a polytropic transformation and neglecting the heat lost with the cylinder wall:

$$T_{TDC}^{EGR} = T_{BDC}^{EGR} \left(\frac{P_{BDC}^{EGR}}{P_{TDC}^{EGR}} \right)^{\frac{1-\gamma}{\gamma}} \quad (26)$$

where γ is the heat capacity ratio of the mixture. Once the piston is at TDC, it is possible to estimate that inside the cylinder will remain a volume of gas corresponding to the clearance volume:

$$V_{TDC}^{EGR} = V_{clear} \quad (27)$$

This is an upper limit, since the volume occupied by valves is not taken into account. All the correlations above allow to estimate the temperature, pressure and volume of EGR, but they do not take into account the change of the mixture composition during this dynamic. To improve the description of the expansion phase, the end gas is treated as a reacting flow in a Plug Flow Reactor (PFR) from BDC