Particle Approximation Approach Applied to Model Diesel Combustion : Application to the HCCI Process.

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Particle approximation has been used to model diesel combustion. The model is based on the IEM model (Interaction by Exchange with the Mean) and takes into account the inhomogeneities (mass and temperature) in the combustion chamber. This includes a reduced mechanism for n-heptane consisting of 25 species and 26 reactions. The aim of this paper is to estimate the minimum number of particles to model the system. The results have shown that for all cases 200 particles are sufficient for diesel engine combustion application. Moreover, we have shown that the hat distribution is not appropriate compared to the normal and lognormal distributions.

1 Introduction

Probability Density Function (PDF) is often chosen to couple chemistry with turbulence for complex reactive flows. When the dimension of the system is high the presumed PDF approach becomes unsuitable and additional PDF transport equations solving approach is used. This last approach is more efficient for nonlinear reaction rates problems and where more than one scalar characterizes the flow [1]. This paper describes a preliminary investigation into the use of the particle approximation of this transport equation approach. The objective is to model Homogeneous Charge Compression Ignition (HCCI) combustion applied to diesel engines with a minimum number of particles, with a view to generalizing this approach to different combustion modes. This paper summarizes the first step of this work focusing on the effects of the initial random distribution and the particle number.

2 Model description

2.1 Dynamical system

The model used here is an IEM model (Interaction by Exchange with the Mean) ([2]), where the fluid within the combustion chamber is represented by a number of computational particles. Each particle evolves function of the rate of change due to the chemical reactions and the mixing term. The chemical reactions term is calculated using a reduced mechanism of n-Heptane oxidation [3] with 25 species and 26 reactions. The evolution of each particle is defined by the following differential system :

$$\dot{\psi_k}^{(i)} = -R_k(\psi^{(i)}) - C(\psi_k^{(i)} - E(\psi_k^{(i)})) \quad \forall k \in \mathcal{K} \quad \forall i \in \mathcal{N}$$

$$\tag{1}$$

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where $\mathcal{K} = \mathcal{S} \cup \{T\}$, \mathcal{S} is the name of all the species and T the temperature, $\mathcal{N} = \{1, \ldots, N\}$ is the set of the particles, $\Psi_k^{(i)}$, $k \in \mathcal{S}$, represents the mass of the species $k \in \mathcal{S}$ of the i^{th} particle and $\Psi_T^{(i)}$ represents the temperature of the i^{th} particle. $R_k(\psi^{(i)})$ represents the evolution of the reactive part of the i^{th} particle and $C = \frac{2}{\tau_r}$ where τ_r is the turbulent time. To solve the equation 1, the expectation is approximated as :

$$E(\psi_k^{(i)}(t)) = \frac{1}{N} \sum_{i' \in \mathcal{N}} \psi_k^{(i')}(t) \quad \forall k \in \mathcal{K} \quad \forall i \in \mathcal{N}$$

$$\tag{2}$$

2.2 Random initial conditions

From the mean initial conditions (mass and temperature) the pseudo-random initial mass of each species of each particle and the pseudo-random initial temperature of each particle have been calculated using three initial distributions. Thanks to these mean values and the distribution law, the other distribution parameters are computed and for each physical size N random pulling are done. Three different distributions have been tested : the normal distribution $\mathcal{N}(\mu, \sigma^2)$, the lognormal distribution $\mathcal{LN}(\mu, \sigma^2)$ and the distribution $\mathcal{C}(\mu, \varepsilon)$, called hat distribution, for which its density has been defined by the following way :

$$f_{\mu,\varepsilon}(x) = \left(\frac{x}{\mu^2 \varepsilon^2} + \frac{\varepsilon - 1}{\mu \varepsilon^2}\right) \mathbb{1}_{[(1-\varepsilon)\mu,\mu]}(x) + \left(-\frac{x}{\mu^2 \varepsilon^2} + \frac{\varepsilon + 1}{\mu \varepsilon^2}\right) \mathbb{1}_{]\mu,(1+\varepsilon)\mu]}(x)$$
$$\forall (x,\mu,\varepsilon) \in \mathbb{R} \times \mathbb{R}^{+*} \times]0,1[$$
(3)

The hat distribution is defined from the parameters μ and ε where ε is used to limit the initial gradients. On another hand, the variance σ^2 of the normal and lognormal distributions has to be calculated to limit the initial gradients. Consequently, σ^2 is solution of the following system :

$$\begin{cases} \text{Find } \sigma^2 > 0 \text{ such that} \\ \mathbb{P}\left(X \in \left] - \infty, \left(1 - \varepsilon\right) \mu\right] \leqslant \delta^- \text{ and} \\ \mathbb{P}\left(X \in \left] (1 + \varepsilon) \mu, +\infty\right] \leqslant \delta^+ \end{cases}$$
(4)

where $\delta^- > 0$ and $\delta^+ > 0$ denote a level error which is fixed by th user (fixed here equal to $\delta^- = \delta^+ = 10^{-9}$).

3 Parametric study

All the numerical results presented in this paper have been done when the engine speed is equal to 1500 rpm during compression and expansion strokes. The initial mean engine parameters are : inlet temperature equal to 350 K, inlet pressure equal to 1.5 bar, EGR rate fixed equal to 20% and the equivalence ratio equal to 0.6. The engine geometry used here is given in the table 1.

Description	Value
Bore	$68.015\ mm$
Connecting rod length	$132.65\ mm$
Stroke	$79.9\ mm$
Compression ratio	11.68:1
Displaced volume	$287.03 \ cm^3$

Table 1: Engine geometry.

3.1 Particle number effects

In order to estimate the minimum number of particles to model the system, several numerical simulations have been done at different particles numbers from 50 up to 10^4 . On another hand, the effects of varying turbulence time scale τ_r , (related to turbulence intensity) have been investigated. In this section, we present the results obtained when the turbulence time scale is very small : $10^{-10} s$ (high turbulence intensity) corresponding to rapid homogeneous mixture and when the turbulence time scale is high : 0.1 s (low turbulence intensity) corresponding to heterogeneous mixture.

Figure (a) shows the in-cylinder pressure evolution for different particle number when the turbulence intensity is high. As expected when the number of particles increases the pressure evolution tends to the curve corresponding to homogeneous case (deterministic approach with the initial conditions equal to the mean operating values (see equation 5)) :

$$\lim_{N \to +\infty} \lim_{\tau_r \to 0} \left(e^{-C \Delta s} \tilde{\psi}_k^{(i)}(s + \Delta s) + \left(1 - e^{-C \Delta s}\right) \frac{1}{N} \sum_{i' \in \mathcal{N}} \tilde{\psi}_k^{(i')}(s + \Delta s) \right) = \mathbb{E}(\psi_k) \quad \forall k \in \mathcal{K}$$
(5)

The relative error plotted in figure (b) shows that the required minimum particle number for homogeneous case is around 200. The same result has been obtained at different engine operating conditions (not shown in this paper).

When the mixture presents inhomogeneities, the results obtained during this study have shown that the same number of particles is sufficient as above (see figures (c) and (d)).

3.2 Initial distribution effects

In this section the effects of initial distribution are studied. Figures (e) and (f) show respectively the results obtained at high and low turbulence intensities for the three distributions. We observe on these figures that the hat distribution is not appropriate for this problem and the normal and the lognormal distributions give the same trends.

4 Conclusion

Particle approximation has been used to model chemistry and turbulence interaction. This work has shown that 200 particles are necessary to model correctly the system with a CPU time around ten minutes. This work has pointed out that the hat distribution is not suitable for this application, it is still under progress in order to model the turbulence time scale.

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(a) Pressure history versus CAD at variable particles number N. Normal distribution, $\tau_r = 10^{-10} s.$



(c) Pressure history versus CAD at variable particles number N. Normal distribution, $\tau_r = 10^{-1} s.$



(e) Temperature history versus CAD for the hat, normal and lognormal distributions. $N=200, \tau_r=10^{-1} s.$



(b) Relative error $(L^1$ -norm) versus N. Normal distribution, $\tau_r = 10^{-10} s$.



(d) Relative error $(L^1$ -norm) versus N. Normal distribution, $\tau_r = 10^{-1} s$.



(f) Temperature history versus CAD for the hat, normal and lognormal distributions. $N=1500,\,\tau_{T}=10^{-10}\,s.$